Metal and Material Physics Division
Fachverband Metall- und Materialphysik (MM)

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Overview of Invited Talks and Sessions

(Lecture halls H10, H22, and H23; Poster P2)

Invited and Topical Talks

MM 2.1	Mon	9:30–10:00	H10	**Probing Ion Migration in ABX_3 Perovskite Compounds: Five Fallacies of Simulations** — •Roger De Souza
MM 5.1	Mon	15:00–15:30	H10	**Room-temperature dislocations in oxide ceramics: from understanding to active engineering** — •Xufei Fang
MM 10.1	Tue	9:30–10:00	H10	**Understanding the impact of disconnection flow on microstructure evolution** — •Marco Salvalaglio
MM 11.1	Tue	10:15–10:45	H10	**The role of disconnections in the shear-migration coupling of grain boundaries** — •Marc Legros, Armin Rajabzadeh, Romain Gautier, Nicolas Combe, Frédéric Mompiou
MM 11.4	Tue	11:30–12:00	H10	**Grain Boundary Spinodals: Faceting Instability and the Role of Junction Energetics** — •Fadi Abdeljawad
MM 11.7	Tue	12:30–13:00	H10	**Atomistic structure of fcc-fcc interface in pure iron and in nanomultilayers: insight from atommistic modeling** — •Helene Zapolsky, Gilles Demange, Yuri Borges Gomes Lima, Anastasiai Titova, Renaud Patte
MM 13.1	Tue	14:00–14:30	H10	**Dynamics of dislocations and grain boundaries during recrystallization of metal nanoparticles** — •Eugen Rabkin, Jonathan Zimmerman
MM 15.1	Wed	9:30–10:00	H10	**Grain Boundary Defect Phases in Thermoelectric Materials: Impact on physical properties** — •Christina Scheu, Ruben Bueno Villoro, Siyuan Zhang, Baptiste Gault, Duncan Zavanelli, Gerald Jeffrey Snyder
MM 16.1	Wed	10:15–10:45	H10	**Microstructure and transport in model isotropic amorphous solids** — •Peter Derlet
MM 16.5	Wed	11:45–12:15	H10	**Structural relaxation and deformation of bulk metallic glasses** — •Gerhard Wilde
MM 19.1	Wed	15:00–15:30	H10	**Structure, interfacial segregation and transformations of solid-state precipitates in aluminium alloys** — •Laure Bourgeois, Nikhil Medhekar, Matthew Weyland
MM 20.1	Wed	15:45–16:15	H10	**Magnetic properties of Fe-based amorphous alloys produced by melt-spinning and selective laser melting** — •Paola Tiberto
MM 20.5	Wed	17:15–17:45	H10	**Diffusion and nucleation in Al-Ni melts using machine-learned MD simulations** — Johannes Sandberg, Leon F. Granz, •Thomas Voigtmann
MM 20.7	Wed	18:00–18:30	H10	**The effect of composition on the thermodynamics, structure, mechanical properties and atomic motion of (Pd-Pt)42.5Cu27Ni9.5P21 alloys** — •Ralf Busch
MM 25.1	Thu	9:30–10:00	H10	**Transformation-induced plasticity in zirconia ceramics: neural network simulations and in-situ experiments** — •David Rodney
MM 33.1	Fri	9:30–10:00	H10	**Fatigue in steels: Micromechanical modelling of cyclic damage** — •Petra Sonnweber-Ribic, Alexandra Stark, Christian Elsässer

Invited Talks of the joint SKM Dissertationspreis 2025 (SYSD)

See SYSD for the full program of the symposium.

SYSD 1.1	Mon	9:30–10:00	H2	**Nanoscale Chemical Analysis of Ferroic Materials and Phenomena** — •Kasper Aas Hunnestad
SYSD 1.2	Mon	10:00–10:30	H2	**Advanced Excitation Schemes for Semiconductor Quantum Dots** — •Yusuf Karli
SYSD 1.3	Mon	10:30–11:00	H2	**Aspects and Probes of Strongly Correlated Electrons in Two-Dimensional Semiconductors** — •Clemens Kuhlenkamp
SYSD 1.4	Mon	11:00–11:30	H2	**Mean back relaxation and mechanical fingerprints: simplifying the study of active intracellular mechanics** — •Till Münker
SYSD 1.5	Mon	11:30–12:00	H2	**Coherent Dynamics of Atomic Spins on a Surface** — •Lukas Veldman

Invited Talks of the joint Symposium AI-driven Materials Design: Recent Developments, Challenges and Perspectives (SYMD)

See SYMD for the full program of the symposium.

SYMD 1.1	Mon	15:00–15:30	H1	**Learning physically constrained microscopic interaction models of functional materials** — •Boris Kozinsky
SYMD 1.2	Mon	15:30–16:00	H1	**GRACE universal interatomic potential for materials discovery and design** — •Ralf Drautz
SYMD 1.3	Mon	16:00–16:30	H1	**Multiscale Modelling & Machine Learning Algorithms for Catalyst Materials: Insights from the Oxygen Evolution Reaction** — •Nong Artrith
SYMD 1.4	Mon	16:45–17:15	H1	**Inverse Design of Materials** — •Hongbin Zhang
SYMD 1.5	Mon	17:15–17:45	H1	**Data-Driven Materials Science** — •Miguel Marques

Invited Talks of the joint Symposium Electronic Structure Theory for Quantum Technology: From Complex Magnetism to Topological Superconductors and Spintronics (SYES)

See SYES for the full program of the symposium.

SYES 1.1	Fri	9:30–10:00	H1	**Ab-initio Design of superconductors** — •Lilia Boeri
SYES 1.2	Fri	10:00–10:30	H1	**Topological superconductivity from first principles** — Bendegúz Nyári, András Lászlóffy, Levente Rózsa, Gábor Csire, Balázs Újfalussy, •László Szunyogh
SYES 1.3	Fri	10:30–11:00	H1	**First-principles study and mesoscopic modeling of two-dimensional spin and orbital fluctuations in FeSe** — •Myrta Grüning, Abyay Ghosh, Piotr Chudzinski
SYES 1.4	Fri	11:15–11:45	H1	**Non-collinear magnetism in 2D materials from first principles: Multiferroic order and magnetoelectric effects.** — •Thomas Olsen
SYES 1.5	Fri	11:45–12:15	H1	**Spin-phonon and magnon-phonon interactions from first principles** — •Marco Bernardi

Sessions

MM 1.1–1.1	Sun	16:00–18:15	H15	**Tutorial: Automated Worksflows (joint session MM/TUT)**
MM 2.1–2.1	Mon	9:30–10:00	H10	**Invited Talk: R. de Souza**
MM 3.1–3.10	Mon	10:15–13:00	H10	**Data-driven Materials Science: Big Data and Worksflows**
MM 4.1–4.11	Mon	10:15–13:00	H22	**Materials for the Storage and Conversion of Energy**
MM 5.1–5.1	Mon	15:00–15:30	H10	**Invited Talk: X. Fang (joint session MM/KFM)**
MM 6.1–6.10	Mon	15:45–18:30	H10	**Phase Transformations**
MM 7.1–7.5	Mon	15:45–17:00	H22	**Materials for the Storage and Conversion of Energy**
MM 8.1–8.5	Mon	17:15–18:30	H22	**Materials for the Storage and Conversion of Energy (joint session MM/KFM)**
MM 9.1–9.74	Mon	18:30–20:30	P1	**Poster**
MM 10.1–10.1	Tue	9:30–10:00	H10	**Topical Talk: M. Salvalaglio**
MM 11.1–11.7	Tue	10:15–13:00	H10	**Topical Session: Defects of Defects**
MM 12.1–12.10	Tue	10:15–13:00	H22	**Materials for the Storage and Conversion of Energy**

MM 13.1–13.5	Tue	14:00–15:30	H10	**Topical Session: Defects of Defects**
MM 14.1–14.5	Tue	14:00–15:15	H22	**Materials for the Storage and Conversion of Energy (joint session MM/KFM)**
MM 15.1–15.1	Wed	9:30–10:00	H10	**Invited Talk: C. Scheu**
MM 16.1–16.8	Wed	10:15–13:00	H10	**Topical Session: Thermophysical Properties of Bulk Metallic Glasses and Bulk Metallic Glass-forming Liquids**
MM 17.1–17.9	Wed	10:15–12:45	H22	**Development of Calculation Methods**
MM 18.1–18.11	Wed	10:15–13:15	H23	**SYMD contributed**
MM 19.1–19.1	Wed	15:00–15:30	H10	**Invited Talk: L. Bourgeois**
MM 20.1–20.7	Wed	15:45–18:30	H10	**Topical Session: Thermophysical Properties of Bulk Metallic Glasses and Bulk Metallic Glass-forming Liquids**
MM 21.1–21.11	Wed	15:45–18:30	H22	**Interface Controlled Properties, Nanomaterials and Microstructure Design**
MM 22.1–22.4	Wed	15:45–16:45	H23	**Materials for the Storage and Conversion of Energy**
MM 23.1–23.5	Wed	17:15–18:30	H23	**Phase Transformations**
MM 24	Wed	18:45–20:45	H10	**Members' Assembly**
MM 25.1–25.1	Thu	9:30–10:00	H10	**Invited Talk: D. Rodney**
MM 26.1–26.6	Thu	10:15–11:45	H10	**Topical Session: Thermophysical Properties of Bulk Metallic Glasses and Bulk Metallic Glass-forming Liquids**
MM 27.1–27.10	Thu	10:15–13:00	H22	**Transport in Materials: Diffusion, Charge or Heat Conduction**
MM 28.1–28.5	Thu	10:15–11:30	H23	**Mechanical properties**
MM 29.1–29.3	Thu	12:00–12:45	H10	**Liquid and Amorphous Materials**
MM 30.1–30.5	Thu	11:45–13:00	H23	**Functional Materials: Performance, Reliability and Degradation; and Complex Materials (joint session MM/KFM)**
MM 31.1–31.11	Thu	15:00–18:00	H10	**Data-driven Materials Science: Big Data and Worksflows**
MM 32.1–32.10	Thu	15:00–17:45	H22	**Transport in Materials: Diffusion, Charge or Heat Conduction**
MM 33.1–33.1	Fri	9:30–10:00	H10	**Invited Talk: P. Sonnweber-Ribic**
MM 34.1–34.7	Fri	10:15–12:15	H10	**Development of Calculation Methods**
MM 35.1–35.6	Fri	10:15–11:45	H22	**Transport in Materials: Diffusion, Charge or Heat Conduction**
MM 36.1–36.10	Fri	10:15–13:00	H23	**Mechanical Properties**
MM 37.1–37.3	Fri	12:00–12:45	H22	**Functional and Complex Materials**

Members' Assembly of the Metal and Material Physics Division

Wednesday 18:45–20:45 H10

MM 1: Tutorial: Automated Worksflows (joint session MM/TUT)

Participants in the tutorial will be able to run all the examples shown in the presentation interactively on their own laptops. There is no need to install any code, just a standard web browser to explore the applications interactively.

Time: Sunday 16:00–18:15 Location: H15

Tutorial MM 1.1 Sun 16:00 H15

Hands-on Tutorial: Automated Workflows and Machine Learning for Materials Science Simulations — •Jörg Neugebauer[1], Tilmann Hickel[2], and Ralf Drautz[3] — [1]MPI für Nachhaltige Materialien, Düsseldorf, Germany — [2]BAM, Berlin, Germany — [3]ICAMS, Ruhr-Universität Bochum, Germany

Machine learning techniques in physics and materials science have revolutionized simulations and experimental analysis. Using these techniques to accurately predict, for example, material properties requires the manipulation and use of vast amounts of data. Manual processing and analysis quickly become impractical and error-prone, so the availability of automated workflows is critical to their efficient, reliable, and consistent application.

In this hands-on tutorial, we provide an interactive, practical introduction to workflow management using Pyiron (www.pyiron.org). Pyiron is an integrated materials science development environment based on Python and Jupyter notebooks that can be used for a wide range of simulation tasks, including rapid prototyping, coupling with experiments, and high-performance computing. The tutorial gives a general introduction to the use of Pyiron with a focus on atomistic simulation tasks. As a practical example, all steps of the workflow for the construction of ab initio phase diagrams will be performed interactively by all participants, e.g. the generation of DFT datasets, the training and validation of machine learning potentials as well as the construction of the phase diagram.

MM 2: Invited Talk: R. de Souza

Time: Monday 9:30–10:00 Location: H10

Invited Talk MM 2.1 Mon 9:30 H10

Probing Ion Migration in ABX_3 Perovskite Compounds: Five Fallacies of Simulations — •Roger De Souza — Institute of Physical Chemistry, RWTH Aachen University, Aachen, Germany

Simulation studies play a central role, in interpreting and explaining experimental data on ion transport, in providing insights at the atomic scale, and in predicting data for new systems. Ion migration in ABX_3 perovskites has been examined with both molecular-static and molecular-dynamic calculations, employing classical pair potentials, reactive force-fields or quantum-mechanical calculations.

In this contribution, taking ion migration in $BaTiO_3$, $CaTiO_3$, and $MAPbI_3$ as examples, I draw attention to problems that may arise when using molecular-static calculations to obtain activation barriers for higher symmetry perovskite phases. In general, a far more critical consideration of simulation results in the literature is required.

MM 3: Data-driven Materials Science: Big Data and Worksflows

Machine Learning, Potential Development

Time: Monday 10:15–13:00 Location: H10

MM 3.1 Mon 10:15 H10

Benchmarking DFT Functionals at Finite Temperature with ASSYST and MLIPs — •Marvin Poul and Jörg Neugebauer — Max-Planck-Institut für Nachhaltige Materialien

A key ingredient to the accuracy of Density Functional Theory (DFT) calculations is the chosen approximation to the exchange-correlation functional. Local Density Approximation (LDA) and Generalized Gradient Approximation (GGA) calculations often bracket experimental observations, but systematic exploration of the behavior of different density functionals is hindered by the high computational cost of DFT in realistic applications, especially concerning finite temperature properties. Using the ASSYST[1] method, we automatically generate unary, general purpose Atomic Cluster Expansion (ACE) Machine Learning Interatomic Potentials (MLIPs) for a range of metals using LDA, PBE and r2SCAN functionals. The key advantage of ASSYST lies in the small cells (≤ 10 atoms per cell) that it generates as training data. This allows us to relabel the data using different functionals very efficiently. We then use these potentials to calculate melting curves, thermal expansion, and formation energies of various defects (grain boundaries, surfaces, point defects) to systematically assess strengths and weaknesses of the DFT functionals. In general, we find good agreement with corresponding DFT results, showing that ASSYST can reliably create transferable potentials for metals at DFT accuracy.

[1]: https://www.researchsquare.com/article/rs-4732459/v1

MM 3.2 Mon 10:30 H10

Assessing the role of physical constraints in machine learning potentials — •Marcel F. Langer, Sergey N. Pozdnyakov, Filippo Bigi, and Michele Ceriotti — Laboratory of Computational Science and Modeling (COSMO) and National Centre for Computational Design and Discovery of Novel Materials (MARVEL), Institute of Materials, École Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland

Machine learning potentials, which approximate the potential energy surface of atomistic systems to enable larger and longer simulations than first-principles methods, have advanced rapidly in recent decades. Much of this development has been driven by the increasingly sophisticated treatment of physical symmetries, in particular invariances, in the underlying machine learning models. However, the rise of so-called unconstrained models, which replace exact invariance with learned approximations, has sparked debate over this approach. Some models even choose to directly predict forces, rendering the resulting force fields non-conservative. We investigate the effectiveness of such models and evaluate the impact of disregarding physical constraints for practical simulations. In particular, we study the effects of breaking rotational symmetry in a machine-learning potential for water [1] and discuss the potential consequences of direct force predictions.

[1]: M.F. Langer, S.N. Pozdnyakov, and M. Ceriotti, Mach. Learn.: Sci. Technol. 5 04LT01 (2024)

MM 3.3 Mon 10:45 H10

Fast and flexible range-separated models for atomistic machine learning — •Philip Loche, Marcel F. Langer, and Michele Ceriotti — Laboratory of Computational Science and Modeling (COSMO), Institute of Materials, École Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland

Most machine learning (ML) interatomic potentials rely on a locality ansatz, decomposing energy into short-ranged, atom-centered contributions. This limits their ability to describe problems dominated by long-range physical effects, such as electrostatics. We present a framework integrating established algorithms for non-bonded interactions – including Ewald summation, PME, and P3M – into atomistic ML.

Reference implementations are provided in PyTorch and JAX. Beyond Coulomb potentials, we introduce Exterior Potential Features for general long-range ML applications. Our modular libraries enable accurate physical force evaluations, seamless integration with local ML schemes via automatic differentiation, and flexible architectures for advanced models. We benchmark these tools for molecular dynamics, range-separated ML potentials, and long-range atomic descriptors.

MM 3.4 Mon 11:00 H10

Beyond Numerical Hessians: Applications for Higher Order Derivatives in Machine Learning Interatomic Potentials — •Nils Gönnheimer[1,2], Karsten Reuter[1], and Johannes T. Margraf[2] — [1]University of Bayreuth — [2]Fritz-Haber-Institut der MPG, Berlin

The development of machine learning interatomic potentials (MLIPs) has revolutionized computational chemistry by enhancing the accuracy of empirical force fields while retaining a large computational speed-up compared to first-principles calculations. Despite these advancements, calculating Hessian matrices remains challenging due to the lack of analytical second-order derivatives, necessitating the use of computationally expensive finite difference methods (which can lead to numerical instabilities because of rounding errors). Automatic differentiation (AD) offers a promising approach to reducing this computational effort and making the calculation of Hessian matrices more efficient and accurate. In this contribution, we discuss the implementation of AD Hessians in the equivariant MACE framework. This new methodology finds applications in screening the heat capacities of metal-organic frameworks (MOFs) and in the calculation of infrared (IR) spectra, which are an ubiquitous tool for molecular characterization.

MM 3.5 Mon 11:15 H10

Diversity-Driven Active Learning of Interatomic Potentials for Reaction Network Exploration — •Francesco Cannizzaro, King Chun Lai, Patricia Poths, Sebastian Matera, Vanessa J. Bukas, and Karsten Reuter — Fritz-Haber-Institut der MPG, Berlin

We present an automatic workflow for the simultaneous active learning of Machine-Learning Interatomic Potentials (MLIPs) and exploration of complex networks of activated events. This workflow consists of alternating periods of training and the generation of candidate structures for the enrichment of the training set using the recently developed Automatic Process Explorer (APE) [1]. This allows us to determine elementary processes and corresponding barriers without the need of human supervision. From the output of the APE explorations, we identify maximally diverse atomic structures utilizing the DECAF fuzzy classification algorithm [2] and add only these to the training set. We exemplify this strategy on carbon intercalation in Pd, using GAP and MACE as MLIP frameworks. We find that this diversity driven approach outperforms state-of-the-art training set designs based on molecular dynamics for finding activated events and corresponding barriers. Particularly, our workflow performs very well in reducing outliers, which is of utmost importance for activated event dynamics since this is often controlled by only a few barriers.

[1] Lai *et al.*, ChemRxiv, https://doi.org/10.26434/chemrxiv-2024-jbzr7 (2024).

[2] Lai *et al.*, J. Chem. Phys. **159**, 024129 (2023).

15 min. break

MM 3.6 Mon 11:45 H10

Accelerating Materials Exploration with Active Machine Learning: Integrating SISSO with FHI-aims — Yi Yao[1,2], Lucas Foppa[1], Akhil Sugathan Nair[1], Andrei Sobolev[1,2], •Konstantin Lion[1,2], Sebastian Kokott[1,2], and Matthias Scheffler[1] — [1]NOMAD Laboratory at the Fritz Haber Institute of the Max Planck Society, Berlin, Germany — [2]Molecular Simulations from First Principles e.V., Berlin, Germany

We present a user-friendly web application for active learning-based materials exploration with the goal of broadening the usability of AI tools. The platform integrates the SISSO (Sure Independence Screening and Sparsifying Operator) method [J. Chem. Phys. 159, 114110 (2023)] with FHI-aims software [Comp. Phys. Commun. 180, 2105 (2009)] to provide interpretable modeling and reliable property predictions. SISSO dynamically updates models during the exploration process, while FHI-aims ensures accurate all-electron density functional theory (DFT)-based calculations. The property prediction workflow is managed using the atomate2 library, providing many "standard" DFT workflows and efficient utilization of compute resources ranging from local machines to cloud infrastructures. By leveraging SISSO-based uncertainty prediction, the application implements active learning to efficiently identify materials with desirable target properties. Two case studies, the exploration of the bulk modulus in perovskites and the prediction of stable oxides under harsh conditions, demonstrate the platform's ability to accelerate materials discovery.

MM 3.7 Mon 12:00 H10

Data-driven design of mechanically hard soft magnetic high-entropy alloys — •Mian Dai[1], Yixuan Zhang[1], Xiaoqing Li[2], Stephan Schönecker[2], Liuliu Han[3], Ruiwen Xie[1], Chen Shen[1], and Hongbin Zhang[1] — [1]Institute of Materials Science, Technical University of Darmstadt, Darmstadt, Germnay — [2]Department of Materials Science and Engineering, KTH - Royal Institute of Technology, Stockholm, Sweden — [3]Max Planck Institute for Sustainable Materials, Düsseldorf, Germany

The rational design of mechanically hard soft magnets, combining high hardness with magnetically soft properties, represents a critical frontier in materials science. Here, we introduce a comprehensive data-driven framework to navigate the vast compositional space of high-entropy alloys (HEAs) and identify candidates optimized for these dual functionalities. Utilizing a curated dataset of 1,842,628 density functional theory calculations, encompassing 45,886 quaternary and 414,771 quinary equimolar HEAs derived from 42 elements, we employ ensemble learning to synergistically integrate multiple predictive models. This methodology captures the relationships between composition, crystal structure, mechanical performance, and magnetic behavior, enabling the identification of alloys with a unique combination of high hardness and magnetic softness. Our framework establishes a robust pathway for the accelerated discovery of next-generation hard-soft magnetic materials, underscoring the transformative potential of data-driven strategies in materials design.

MM 3.8 Mon 12:15 H10

Autonomous optimization of coin-cell batteries and thin-film growth — •Edan Bainglass[1,6], Peter Kraus[2,5], Francisco Ramirez[3,6], Enea Svaluto-Ferro[2], Loris Ercole[3,6], Benjamin Kunz[2], Sebastiaan Huber[3,6], Nukorn Plainpan[2], Nikita Shepelin[1], Nicola Marzari[1,3,6], Corsin Battaglia[2,3,4], and Giovanni Pizzi[1,3,6] — [1]PSI, Villigen, Switzerland — [2]Empa, Dübendorf, Switzerland — [3]EPFL, Lausanne, Switzerland — [4]ETH Zurich, Zurich, Switzerland — [5]TUB, Berlin, Germany — [6]MARVEL, Switzerland

Advancements in materials science are increasingly driven by the integration of automation of both experiments and simulations, machine learning, and robust data management frameworks. In this talk, we discuss the integration of experimental systems with the AiiDA [1] workflow management system, both battery coin cell assembly and cycling [2], and for thin film growth by pulsed laser deposition (PLD). We discuss the ongoing integration of these platforms with the FINALES [3] fast intention-agnostic learning server towards fully autonomous optimization of battery end-of-life (EOL) performance. We also discuss preliminary results demonstrating the feasibility of autonomously optimizing the layer-by-layer thin-film growth with PLD. These case studies demonstrate the potential of automated workflows to accelerate the discovery and optimization of functional materials.

[1] S. P. Huber et al., Sci. data 7, 300 (2020)

[2] P. Kraus et al., J. Mat. Chem. A 12, 10773 (2024)

[3] M. Vogler et al. Adv. Ener. Mat. 2403263 (2024)

MM 3.9 Mon 12:30 H10

Learning Disorder in Generative Materials Discovery - Bridging Prediction and Experiment — •Konstantin Jakob[1], Aron Walsh[2], Karsten Reuter[1], and Johannes T. Margraf[1,3] — [1]Fritz-Haber-Institut der MPG, Berlin, Germany — [2]Imperial College London, London, UK — [3]University of Bayreuth, Bayreuth, Germany

In recent years, generative machine learning (ML) models have demonstrated tremendous potential for the design and discovery of new materials. This has led to extensive predictions of previously unknown, potentially stable inorganic materials. However, current models suffer from the fact that the underlying training data is purely based on density functional-calculations for small, ideal crystals. As a consequence, many of the supposedly new materials are in fact experimentally known as disordered crystals. In this work, we address this issue by performing a thorough analysis of crystal disorder in the experimental structures of the Inorganic Crystal Structure Database (ICSD). Based on this, we develop disorder classification models and representations that can predict the likelihood of disorder across chemical space. Eventually, these concepts will allow us to extend current generative models to realistic crystal systems and bridge the gap between prediction and experiment.

MM 3.10 Mon 12:45 H10

Materials-Discovery Workflows Guided by Symbolic Regression: Identifying Stable Oxides for Catalytic Applications — •Akhil S. Nair, Lucas Foppa, and Matthias Scheffler — The NOMAD Laboratory at the FHI of the Max Planck Society, Berlin, Germany

AI-driven workflows will accelerate materials discovery by efficiently guiding experiments or simulations towards materials with desired properties. However, probabilistic AI approaches commonly used in these workflows are limited by the relatively small size of high-quality datasets and they rely on typically unknown, low-dimensional representations. Herein, we discuss the recent advancements in applying symbolic regression based on the sure-independence screening and sparsifying operator (SISSO) approach within iterative frameworks for materials discovery. This involves an ensemble approach for the uncertainty quantification of SISSO models as well as the development of optimization strategies to efficiently explore promising regions of the materials space. These developments present an opportunity to integrate SISSO into sequential-learning workflows for materials discovery. Importantly, SISSO provides materials-property maps covering the entire materials space, further reducing the risk that the workflow misses promising materials that were overlooked in the initial dataset. We demonstrate the effectiveness of the SISSO-guided workflows by identifying stable oxides for catalytic applications.

MM 4: Materials for the Storage and Conversion of Energy

Metal Hydrides, Hydrogen Embrittlement

Time: Monday 10:15–13:00 Location: H22

MM 4.1 Mon 10:15 H22

Atomic cluster expansion potential for the palladium hydride system — •Minaam Qamar[1], Apinya Ngoipala[2], Matous Mrovec[1], and Matthias Vandichel[2] — [1]ICAMS, Ruhr-University Bochum, Germany — [2]Department of Chemical Sciences and Bernal Institute, University of Limerick, Ireland

Palladium (Pd) is extensively studied for metal-hydrogen interactions due to its remarkable ability to absorb large amounts of hydrogen under standard temperature and pressure conditions, forming stable palladium hydride structures. This property makes Pd a critical material for various hydrogen-related applications, including hydrogen storage and as a catalyst for hydrogen evolution reactions. We developed a highly accurate and computationally efficient Atomic Cluster Expansion (ACE) potential to unravel atomistic insights into the Pd-H interaction. This potential was utilized to perform molecular dynamics and Monte Carlo simulations, providing a detailed understanding of the formation mechanisms of palladium hydride nanoclusters and bulk structures.

MM 4.2 Mon 10:30 H22

Hydrogen kinetics in HPT-deformed bulk Mg and Mg-based alloys — •Giorgia Guardi[1], Sabine Schlabach[1,2,3], Julia Ivanisenko[2], Stefan Wagner[1], and Astrid Pundt[1] — [1]Karlsruhe Institute of Technology (KIT), Institute for Applied Materials (IAM-WK), Karlsruhe, Germany — [2]Karlsruhe Institute of Technology (KIT), Institute of Nanotechnology (INT), Karlsruhe, Germany — [3]Karlsruhe Institute of Technology (KIT), Karlsruhe Nano Micro Facility (KNMFi), Karlsruhe, Germany

Magnesium (Mg) is a light and abundant element that can store hydrogen with a gravimetric density of 7.6 wt. % and a volumetric density of 110 kgH/m^3. Therefore, it is a highly promising hydrogen storage material for a sustainable energy economy. However, its technical use is hindered by an inherent kinetic blockade in magnesium hydride. A high content of grain boundaries is expected to improve hydrogen kinetics in Magnesium samples, particularly in the magnesium hydride phase. This can be achieved in bulk samples through the use of severe plastic deformation techniques, such as High-Pressure Torsion (HPT).

High-pressure torsion is not fully effective in reducing the grain size in pure bulk magnesium due to dynamic recrystallization. To overcome this lower limit to bulk magnesium grain size, Mg- 2.3 at.% Zn- 0.17 at. % Zr alloys are used, reaching a final grain size of approximately 100 nm after HPT. This study examines the impact of the sample's microstructure on hydrogen kinetics. Hydrogen absorption is studied at room temperature by gas-phase and electrochemical hydrogen loading.

MM 4.3 Mon 10:45 H22

A first principles study on the free energy landscape of chemisorbed hydrogen atoms on a Pt (111) surface modified by transition metals — •Bingxin Li, Sudarsan Surendralal, Mira Todorova, and Jörg Neugebauer — Max-Planck-Institut für Nachhaltige Materialien GmbH, Max-Planck-Straße 1, 40237 Düsseldorf

Platinum (Pt) is considered an excellent catalyst for the hydrogen evolution reaction (HER) due to its optimal hydrogen binding strength, as suggested by the Sabatier principle and the volcano plot of the HER. In surface-catalysed electrochemical reactions, the incorporation of adsorbates or dopants into a host surface can significantly enhance the catalytic selectivity, activity, and stability compared to the pristine surface while also introducing some novel properties not observed on the parent surfaces. Transition metals (TMs), such as Cu, Ag, Au, Pd, Ru, Rh, and Ir, form metal-hydrogen bonds with unique characteristics, resulting in varied H adsorption patterns and distinct hydrogen evolution behaviours. Consequently, doping these transition metals into a Pt (111) surface can significantly alter its catalytic properties for the HER, either by modifying H adsorption configurations or by impacting the reaction barrier of the fundamental steps for the hydrogen evolution, though the underlying mechanisms remain unclear. To this end, we employ ab initio molecular dynamics (AIMD) simulations to investigate H adsorption on TM-doped Pt (111) surfaces in the presence/absence of explicit water by constructing laterally resolved free energy maps of chemisorbed H atoms.

MM 4.4 Mon 11:00 H22

Local hydrogen concentration and distribution in Pd nanoparticles: An in-situ STEM-EELS approach — •Svetlana Korneychuk[1,2], Stefan Wagner[1], Darius Rohleder[3], Philipp Vana[3,4], and Astrid Pundt[1] — [1]IAM-WK, Karlsruhe Institute of Technology — [2]Karlsruhe Nano Micro Facility (KNMFi), Karlsruhe Institute of Technology — [3]Institute of Physical Chemistry, Georg-August-University Göttingen — [4]Wöhler Research Institute for Sustainable Chemistry (WISCh), Georg-August-University Göttingen

Local detection of hydrogen concentration in metals is of central importance for many areas of hydrogen technology, such as hydrogen storage, detection, catalysis, and hydrogen embrittlement. We demonstrate a novel approach to measure the hydrogen concentration in a model system consisting of cubic palladium nanoparticles, with a lateral resolution down to 4 nm. By measuring the shift of the Pd bulk plasmon peak with scanning transmission electron microscopy combined with energy electron loss spectroscopy during in-situ hydrogen gas loading and unloading, local detection of the hydrogen concentration is achieved in TEM [1]. With this method, concentration changes inside the NPs at various stages of hydrogenation/dehydrogenation are observed with nanometer resolution. The versatility of in-situ TEM allows to link together microstructure, hydrogen concentration and local strain, opening up a new chapter in hydrogen research. [1] S. Korneychuk, et al., 'Local hydrogen concentration and distribution in Pd nanoparticles: An in-situ STEM-EELS approach', Small, accepted

MM 4.5 Mon 11:15 H22

Hydride formation in open thin film metal hydrogen systems: Cahn-Hilliard-type phase-field simulations coupled to elasto-plastic deformations — •Stefan Wagner[1], Alexander Dyck[2], Johannes Gisy[2], Frederik Hille[2], Astrid Pundt[1], and Thomas

Böhlke[2] — [1]Institute for Applied Materials (IAM-WK), Karlsruhe Institute of Technology (KIT), Germany — [2]Institute of Engineering Mechanics (ITM), Karlsruhe Institute of Technology, Germany

Metal-hydrogen systems are versatile model systems to study alloy thermodynamics and structural phase transitions. Hydrogen absorption and hydride formation in metals induce a volume expansion of the metal, leading to incompatibility stresses at internal and external interfaces. Resulting changes of the thermodynamic stability of phases in response to the mechanical constraint conditions can be understood by investigating the chemo-mechanical coupling [1,2]. Utilizing niobium-hydrogen thin films, combining a Cahn-Hilliard type phase-field theory and Finite-Element-Modeling (FEM) we study the feedback-loop of the local stress state, elasto-plastic deformations and hydrogen diffusion, determining the driving force of precipitation and growth of the hydride phase under open-system conditions. The simulation results are informed by and compared to measurements of the concentration-dependent stress state, chemical potential and phase separation in epitaxial niobium-hydrogen thin films adhered to sapphire substrates [3]. [1] A. Dyck, T. Böhlke, A. Pundt, S. Wagner, Scr. Mat. 247 (2024) 116117. [2] A. Dyck et al., Scr. Mat. 251 (2024) 116209. [3] A. Dyck et al., accepted to Mech. of Mat.

MM 4.6 Mon 11:30 H22

Hydrogen: a catalyst for abnormal grain growth in inert-gas condensed nanocrystalline Pd-Au? — •Fabian Andorfer[1], Jules M. Dake[1], Markus Ziehmer[1], Johannes Wild[2], Torben Boll[2], Dorothée Vinga Szabó[2], Stefan Wagner[2], Astrid Pundt[2], and Carl E. Krill III[1] — [1]Institute of Functional Nanosystems, Ulm University — [2]Institute of Applied Materials - Materials Science and Engineering (IAM-WK), Karlsruhe Institute of Technology

Heat treatment causes some polycrystalline materials to manifest abnormal grain growth (AGG), during which a few grains acquire a significant growth advantage compared to the remaining matrix grains, resulting in a bimodal distribution of grain sizes. Inert-gas condensed nanocrystalline Pd-Au alloys undergo an extreme form of AGG. This system is known to absorb hydrogen. When Pd-Au alloys are exposed to hydrogen below a certain gas pressure, hydrogen atoms primarily occupy grain boundaries and interstitial sites. This segregation is expected to lower the excess energy of the grain boundaries, which should have a noticeable effect on subsequent grain growth. To test this, Pd-Au samples were heat treated in argon and hydrogen atmospheres, respectively. The average size of the abnormally grown grains was determined, and the grain shape was characterized by calculating the circularity. Hydrogen appeared to increase the rate of abnormal grain “nucleation” without affecting the resulting grain shape.

MM 4.7 Mon 11:45 H22

The liquid intermediate phase for a hydrogen storage material — •Anastasiia Thase[1], Oliver Alderman[2], Chiara Milanese[3,4], Alessandro Girella[4], Claudio Pistidda[5], Martin Müller[5,6], and Sebastian Busch[1] — [1]GEMS MLZ, Helmholtz-Zentrum Hereon WPN — [2]ISIS Neutron and Muon Source — [3]C.S.G.I. Department of Chemistry, Physical Chemistry Division, University of Pavia — [4]Pavia Hydrogen Lab — [5]Helmholtz-Zentrum Hereon WTN — [6]CAU zu Kiel, Leibnitzstr. 19, 24098 Kiel, Germany

Hydrogen storage in light hydrides for mobile applications is a widely discussed but a highly controversial topic because of its ability to form explosive mixtures with oxygen. However, this danger is eliminated, if hydrogen is stored in complex hydrides, which provide hydrogen only under significant heat impact.

The main issue for complex hydride mixtures is the kinetics of the reversible reaction with hydrogen. One of prospective candidates is $6Mg(NH_2)_2$:9LiH, which promptly interacts with hydrogen when doped with $LiBH_4$. Its catalytic impact is explained by the formation of low-melting intermediate phases with high Li-ion conductivity: a metastable $Li_2BH_4NH_2$ and a peritectically melting $Li_4BH_4(NH_2)_3$.

In the $LiNH_2 - LiBH_4$ phase diagram, the eutectic point is located at the 1:2 ratio and 90^{o}C. This eutectic mixture was characterized by various techniques, including neutron total scattering, and its intrinsic structure under the reaction conditions was elucidated by EPSR, which gave a hint about its role as a liquid-phase catalyst in the corresponding hydrogen storage composition ($6Mg(NH_2)_2$:9LiH:6$LiBH_4$).

MM 4.8 Mon 12:00 H22

Machine Learning Interatomic Potentials for Studying Hydrogen Storage in TiCr2 Laves Phase Alloys — •Pranav Kumar, Blazej Grabowski, and Yuji Ikeda — Institut für Materialwissenschaft, Universität Stuttgart, Pfaffenwaldring 55, 70569 Stuttgart, Germany

Efficient hydrogen storage is a crucial challenge for the widespread absorption of hydrogen as a clean energy carrier. TiCr2 Laves phase alloys, with their exceptional hydrogen absorption and diffusion properties, represent a promising class of materials for this purpose. This study employs a multiscale computational strategy, integrating density functional theory (DFT) and machine learning interatomic potentials (MLIPs), to investigate hydrogen behavior in TiCr2 Laves phases. Key areas of focus include hydrogen binding energies, diffusion pathways, and the complex effects of hydrogen clustering, which influence storage capacity and transport. Notably, our findings reveal possible equilibrium hydride structures consistent with experimental observations, offering valuable validation of the computational models. By leveraging large-scale DFT simulations within an active learning framework, we develop accurate MLIPs that enable efficient exploration of the phase space across diverse hydrogen concentrations. These MLIPs bridge atomic-scale simulations, facilitating precise calculations of hydrogen diffusion coefficients and shedding light on the mechanisms of hydrogen mobility. The insights derived from this work enhance our understanding of hydrogen-metal interactions and provide critical information for optimizing hydrogen storage materials.

MM 4.9 Mon 12:15 H22

The impact of Mn and Al on the trapping and diffusion of hydrogen in γ-Fe: An atomistic insight — •Bikram Kumar Das[1], Poulami Chakraborty[1], Mauricio Rincón Bonilla[1], and Elena Akhmatskaya[1,2] — [1]Basque Center for Applied Mathematics, Bilbao, Spain — [2]Ikerbasque - Basque Foundation for Science, Spain

We propose a first principles-based framework to systematically unlock the physical underpinnings of local distribution of the solute atoms on hydrogen trapping and diffusion in Mn/Al-alloyed γ-Fe. In our scheme, all thermodynamically stable substitutional solute sites were identified ($<=$ 5.4 wt% Mn; $<=$ 4 wt% Al) up to the third nearest neighbour (NN) shell of a single H atom. The impact of Mn/Al on H-binding was quantitatively evaluated, indicating a surprisingly strong correlation with the local Al distribution regardless Mn content, and indirect stabilization by Al when present in the 2nd NN shell. Nonetheless, Al strongly repels H bonding. The contradictory role of Al was explained in terms of bonding/anti-bonding orbitals occupancy in H-M interactions (M = Al, Mn, Fe). The barriers to H hopping between adjacent local environments and the corresponding jump frequencies were subsequently calculated, providing insights into the limits imposed by the presence of Al and Mn on H mobility in Mn/Al-alloyed γ-Fe. Most notably, presence of Al in the 2nd NN shell of H severely reduces the H jump frequency, leading to irreversible trapping at high Al contents. Such behaviour may critically contribute to mitigate H-induced delayed fracture in Al-rich austenite steel.

MM 4.10 Mon 12:30 H22

Hydrogen - Microstructure Interaction in Ferritic Steels: From Ab-initio Simulations to Experiments — •Onur Can Şen[1,2,3], Santiago Benito[2], Sebastian Weber[2], and Rebecca Janisch[3] — [1]IMPRS SusMet, Max Planck Institute for Sustainable Materials, Germany — [2]Institute for Materials, Chair of Materials Technology, Ruhr-University Bochum, Germany — [3]ICAMS, Ruhr-University Bochum, Germany

Hydrogen embrittlement (HE) is a phenomenon where hydrogen negatively impacts the mechanical properties of metallic materials. Mitigating HE requires minimizing hydrogen diffusion in microstructures and understanding how local heterogeneities influence this process across different length scales. While advanced experimental and computational methods exist, their application to varying systems complicates model validation. To address this, simplified ferritic Fe-based alloys were produced, and subjected to thermomechanical treatments, and their microstructures were characterized using EBSD. This approach aims to assess the hydrogen storage capacities of microstructural heterogeneities and their influence on the effective diffusion coefficient. Complementary ab initio density functional theory calculations were performed to evaluate hydrogen trapping energies and diffusion barriers under different chemical environments and CSL boundaries. These calculations inform predictions of hydrogen solubility and distribution within the experimental microstructures, to be validated experimentally. This work shows the importance of combining simulations and experiments to understand microstructural heterogeneities’ role in HE.

MM 4.11 Mon 12:45 H22

Hydrogen Embrittlement in fatigue damage of ferritic steel: Theoretical investigation of failure mechanisms in varying hydrogen environments — •Alexandra Stark[1,2], Petra Sonnweber-Ribic[1], and Christian Elsässer[2] — [1]Robert Bosch GmbH, CR, 71272 Renningen — [2]Fraunhofer IWM, 79108 Freiburg

In this theoretical study, the influence of hydrogen on the fatigue behavior of a ferritic steel is examined by using a coupled hydrogen-diffusion and crystal-plasticity finite-element (CPFE) model. The damaging effect of hydrogen on structural materials, particularly ferritic and martensitic steels, poses a significant challenge for a wide range of technical applications. Despite being known for about 150 years, the underlying mechanisms of hydrogen embrittlement remain the subject of scientific debates. CPFE models are suitable for ensuring a microstructure-sensitive modelling and enabling the description of local plastic deformation, both essential factors in the complex process of metal fatigue. The presented study investigates the individual and combined effects of different damage models based on proposed hydrogen embrittlement failure mechanisms [1]. Furthermore, the work explores the impact of diverse environmental conditions on the cyclic material damage. The effects of varying local hydrogen concentration and distribution on the fatigue damage, as implemented in the CPFE model, are examined and discussed. [1] A. Stark, P. Sonnweber-Ribic, and C. Elsässer, Theoretical study of individual and combined effects of HELP- and HEDE-based damage models on the fatigue behavior of ferritic steel by hydrogen, submitted (2024).

MM 5: Invited Talk: X. Fang (joint session MM/KFM)

Time: Monday 15:00–15:30 Location: H10

Invited Talk MM 5.1 Mon 15:00 H10

Room-temperature dislocations in oxide ceramics: from understanding to active engineering — •Xufei Fang — Institute for Applied Materials, Karlsruhe Institute of Technology, Karlsruhe, Germany

In the conventional picture, dislocations are most relevant for metals while ceramics are considered brittle and exhibit little or no plasticity at room temperature. However, recent years' research on dislocations in ceramics suggests that dislocations may have been much under-appreciated in ceramics. Proofs-of-concept for dislocation-tuned functional properties suggest that dislocations may hold great technological potential in advanced ceramics. As the prerequisite to harvest dislocation-tuned properties, engineering dislocations into ceramics without brittle fracture has thus become a pressing bottleneck. To tackle this challenge, we have separately examined the dislocation behavior including dislocation nucleation, multiplication and motion, enabling us to tune dislocations into ceramic oxides at room temperature. We can now achieve a dislocation density up to ~10^15/m^2 with a plastic zone size of up to milli-/centimetres using a mechanical deformation toolbox. We further extend the material toolbox by discovering and reporting more oxide perovskites that can be plastically deformed at room temperature across the length scale. The combined deformation and material toolboxes offer a new platform for studying the dislocation-tuned functional properties (e.g., electrical and thermal conductivity) and the mechanical properties (such as plasticity, toughness, and damage tolerance) over a wide range of length scales.

MM 6: Phase Transformations

Time: Monday 15:45–18:30 Location: H10

MM 6.1 Mon 15:45 H10

Phase transitions in 2D halide perovskites using machine learned potentials — •Erik Fransson, Julia Wiktor, and Paul Erhart — Chalmers University of Technology, Gothenburg, Sweden

Hybrid halide perovskites are a promising class of materials for various applications, including high-efficiency solar cells, lasers, and light-emitting diodes. So-called two-dimensional (2D) halide perovskites, composed of a small number of perovskite layers stacked on top of each other and separated by organic cations that act as spacers, have much improved stability compared to their 3D counterparts. Here, we focus on the prototypical perovskite methylammonium lead halide (MAPI), and demonstrate that the dimensionality of these 2D materials and the choice of organic linker molecules can have a strong impact on phase transitions in these systems. This is investigated through large-scale molecular dynamics simulations using machine-learned potentials. We analyze the phase transition temperatures and characteristics with varying numbers of perovskite layers to understand how the transition properties change as a function of the system's dimensionality. For a larger number of perovskite layers, the 3D bulk phase transition temperature is recovered, whereas, for only a few perovskite layers, the phase transition temperature shifts up by about 100 K. Additionally, we observe surface effects, such as the surface layers (closest to the organic linker) exhibiting stronger octahedral tilting and undergoing phase transitions at higher temperatures (about 100 K) compared to the interior bulk layers.

MM 6.2 Mon 16:00 H10

Quantum phase diagram of sulfure hydride — •Marco Cherubini and Michele Casula — IMPMC, CNRS, Paris, France

In the recent rush towards room temperature superconductivity, hydrogen-based materials are the most prosiming candidates. Sulfulr hydride exhibits a maximum superconductive critical temperature of about 200K at 150 GPa. To our knowledge, a comprehensive theoretical characterization of the phase diagram of sulfur hydride in a wide temperature range is still missing in literature. To address this, we performed path integral molecular dynamics simulations (PIMD). The description of the low temperature regime has been made feasible by the use a machine learning potential trained on ab-initio data. We found three different regimes. At high pressure, the phase diagram is dominated by a paraelectric phase, with symmetric hydrogen bonds. Reducing the pressure, we observed first a regime characterized by finite local dipole moments and finally, at even lower pressures, the ferroelectric regime. Quantum simulations show that the formation of finite local moments is temperature-independent, unlike the transition to the ferroelectric regime. Classical simulations, by contrast, showed stronger temperature dependence for both the transitions and significantly higher critical pressures, highlighting the impact of quantum nuclear fluctuations.

MM 6.3 Mon 16:15 H10

Magnetic-field induced phase transition crossover in the triangular-lattice antiferromagnet: Ba_3CoSbO_9 — •Sanjay Kumar[1], Koushik Chakraborty[2], Aditi Agrawal[2], Shalini Mishra[3], M. P. Saravanan[2], Arvind Kumar Yogi[2], Satyapal S. Rathore[4], and Rashi Nathawat[1] — [1]Functional Ceramics and Smart Materials Lab, Department of Physics, Manipal University Jaipur, Jaipur - 303007, India — [2]UGC-DAE Consortium for Scientific Research, University Campus, Khandwa Road, Indore-452001, India — [3]Department of Physics, Govt. Holkar Science College, Indore (M.P.) 452001, India — [4]Department of Physics, Cluster University of Jammu, Jammu * 180001, India

We report magnetic and structural properties of triangular-lattice antiferromagnet Ba_3CoSbO_9 by means of x-ray diffraction (XRD), magnetic susceptibility, specific heat, x-ray photoelectron spectroscopy (XPS), and dielectric measurements. Thermodynamic measurements show a long-range ordered (LRO) state at Néel temperature $T_N = 3$ K which was found to be shift at higher temperatures at about $T_N = 4.1$ K under the higher magnetic fields. Moreover, we have found higher Curie-Weiss temperature $\theta_{\mathrm{CW}} \sim$-133.2 K from the inverse susceptibility fit which reveals frustration parameter about 44, suggesting magnetic lattice is highly frustrated. Further, a spin-glass state signature was evident at around 6.5 K, which was found to be fully suppressed at a higher magnetic field (H ∼16 T). Interestingly, Ba_3CoSbO_9 exhibits a broad maximum at around T_{max} ∼5 K which becomes pronounced as the magnetic field is increased.

MM 6.4 Mon 16:30 H10

Anomalous spin-lattice coupling in the quasi-one-dimensional spin-1 corrugated skew-chain antiferromagnet: $Ni_2V_2O_7$ — •Arvind Kumar Yogi[1], Hemant Singh Kunwar[1], Koushik Chakraborty[1], Aditi Agrawal[1], Binoy Krishna De[1], Pragati Sharma[1], Shalini Mishra[2], D. T. Adroja[3], Mayanak Kumar Gupta[4], R. Mittal[4], R. Venkatesh[1], and V. G. Sathe[1] — [1]UGC-DAE Consortium for Scientific Research, University Campus, Khandwa Road, Indore-452001, India — [2]Department of Physics, Govt. Holkar Science College, Indore (M.P.) 452001, India — [3]ISIS Neutron and Muon Facility, STFC, Rutherford Appleton Laboratory, Chilton, Oxfordshire OX11 0QX, United Kingdom — [4]Solid State Physics Division, Bhabha Atomic Research Centre, Trombey, Mumbai-400005, India

We report spin-lattice coupling through detailed structural, magnetic, and lattice-dynamics studies of the $S = 1$ quasi-one-dimension lattice $Ni_2V_2O_7$ compound. Our susceptibility χ (T) and heat capacity measurements (C_P/T) measurement conclusively show that the antiferromagnetic transition occurs at $T_{N1} = \sim 6.7$ K and $T_{N2} = \sim 5.8$ K. From detailed lattice dynamics, two Raman mode showed anomalous lattice softening below ∼100 K due to Ni dimerization as supported by ordering of the J_1 exchange interaction. Importantly, the spin-lattice coupling has been established below ∼100 K and the spin-lattice coupling constant (λ_{sp}) for various Raman modes has been deduced which shows multiferroic behaviour below T_{N1}. In addition, the detailed study of lattice dynamics by first principle calculation is presented.

MM 6.5 Mon 16:45 H10

Chirality in the Kagome Metal CsV_3Sb_5 — H.J. Elmers[1], O. Tkach[1], Y. Lytvynenko[1], P. Yogi[1], M. Schmitt[2,3], D. Biswas[2], J. Liu[2], S.V. Chernov[4], Q. Nguyen[5], M. Hoesch[4], D. Kutnyakhov[4], N. Wind[4,6], L. Wenthaus[4], M. Scholz[4], K. Rossnagel[4,6], A. Gloskovskii[4], C. Schlueter[4], A. Winkelmann[7], A.-A. Haghighirad[8], T.-L. Lee[2], M. Sing[3], R. Claessen[3], M. Le Tacon[8], J. Demsar[1], G. Schönhense[1], and •O. Fedchenko[1] — [1]JGU Mainz, Germany — [2]DIAMOND, Didcot, United Kingdom — [3]Physikalisches Institut Würzburg, Germany — [4]DESY, Germany — [5]SLAC, Menlo Park, USA — [6]CAU Kiel, Germany — [7]University of Krakow, Poland — [8]KIT, Karlsruhe, Germany

Using x-ray photoelectron diffraction (XPD) and angle-resolved photoemission spectroscopy, we study photoemission intensity associated with the changes in the geometric and electronic structure of the kagome metal CsV_3Sb_5 upon transition to an unconventional charge density wave (CDW) state. The XPD patterns reveal the presence of a chiral atomic structure in the CDW phase. Using circularly polarized x-rays, we have found a pronounced non-trivial circular dichroism in the angular distribution of the valence band photoemission in the CDW phase, indicating a chirality of the electronic structure. This observation is consistent with the proposed orbital loop current order. The results suggest an antiferromagnetic coupling of the orbital magnetic moments along the c-axis.

[1] H.J. Elmers et al., e-print on arXiv, 2408.03750 (2024).

15 min. break

MM 6.6 Mon 17:15 H10

Pressure-temperature phase diagram of calcium using quantum-accurate finite-temperature free energies — •Raynol Dsouza[1], Marvin Poul[1], Liam Huber[2], and Jörg Neugebauer[1] — [1]Max Planck Institute for Sustainable Materials, Düsseldorf, Germany — [2]Grey Haven Solutions, Vancouver, Canada

Pure calcium has been experimentally shown to exhibit several stable phases across a range of high pressures. While many of these phases have been theoretically predicted using T=0 K ab inito calculations [1], the relative stability of the distorted simple cubic phases above 30 GPa at finite temperatures remains unclear. To address this ambiguity, we developed an Atomic Cluster Expansion (ACE) potential [2] for calcium, fitting it to a structural dataset generated using the ASSYST methodology outlined in [3]. Quantum-accurate finite-temperature free energies were determined using the Temperature Remapping Approximation (TRA) [4]. The resulting pressure-temperature phase diagram offers new insights into the phase stability of calcium at elevated pressures and temperatures.

[1] Ishikawa et al., https://doi.org/10.1103/PhysRevB.81.092104 [2] Bochkarev et al., https://doi.org/10.1103/PhysRevMaterials.6.013804 [3] Poul et al., https://doi.org/10.21203/rs.3.rs-4732459/v1 [4] Dsouza et al., https://doi.org/10.1103/PhysRevB.105.184111

MM 6.7 Mon 17:30 H10

Phase-stability Study of the Marcasite-Structure Solid Solutions (Fe, TM)Sb_2 (TM = Cr, Ni) Synthesized via Combinatorial Co-Deposition and Antimonization — •Martin Kostka[1], Luqman Mustafa[1], Maik Golombiewski[1], Jill Fortmann[2], Aurelija Mockute[2], Alan Savan[2], Alfred Ludwig[2], Adreas Kreyssig[1], and Anna Böhmer[1] — [1]Experimental physics IV, Ruhr University Bochum, 44801 Bochum — [2]Materials Discovery and Interfaces, Institute for Materials, Ruhr University Bochum, 44801 Bochum

Transition-metal di-pnictides of the pyrite-marcasite family are model systems for crystal chemistry. We investigate phase formation and stability of transition-metal di-antimonides in the orthorhombic marcasite structure. We employ a two-step synthesis of granular films, using combinatorial co-deposition of the transition metals and subsequent antimonization at different temperatures. This technique allows efficient exploration of substitution ranges and lattice parameter evolution within the marcasite structure. We investigate the formation and crystal structures of the (Fe,Ni)Sb_2 and (Fe,Cr)Sb_2 substitution series. We evidence the continuous substitution of $FeSb_2$ (class A marcasite) with Ni up to $Fe_{0.5}Ni_{0.5}Sb_2$, and a clear phase separation between $Fe_{0.5}Ni_{0.5}Sb_2$ and a Ni-rich $Ni_{1-z}Fe_zSb_2$ phase (class B marcasite). Cr-substituted $FeSb_2$ shows a subtle phase separation into an Fe-rich $Fe_{1-y}Cr_ySb_2$ and a Cr-rich $Cr_{1-z}Fe_zSb_2$-phase (both class A marcasite) when synthesized at 500°C, but not at higher Temperatures. We acknowledge support from DFG (TRR288,A02).

MM 6.8 Mon 17:45 H10

Investigation of glass formation in Pd40Ni40P20 metallic glass via fast scanning calorimetry — •Hongshuai Li, Sher Bahadur Raut, and Gerhard Wilde — Institute of Materials Physics, University of Münster, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany

Pd-Ni-P metallic glasses (MGs) exhibit exceptional glass-forming ability; in fact, Pd40Ni40P20 was the first bulk metallic glass-forming alloy discovered. Understanding glass formation in these materials requires exploring factors that impede correlated atomic motions in glass-forming liquids. This study investigates the atomic relaxation and thermal history of Pd40Ni40P20 MG, utilizing data from multiple cycles of heating around the glass transition temperature, activation energy determined by flash differential scanning calorimetry (DSC), and critical cooling rates. Additionally, we examine the effects of annealing time on the DSC signals at high heating rates of up to 1000 K/s. Our results demonstrate that adjustments in cooling rates and annealing duration significantly influence glass transition behavior and thermal stability. These findings enhance our understanding of the mechanisms underlying glass formation in Pd-Ni-P MGs and their potential applications in advanced materials.

MM 6.9 Mon 18:00 H10

Tuning excitonic transition by Cr doping and associated lattice softening in the vdW chalcogenide: Ta2NiSe5 — •Isha Isha[1], Koushik Chakraborty[1], Aditi Agrawal[1], M. Isobe[2], and Arvind Kumar Yogi[1] — [1]UGC-DAE Consortium for Scientific Research, University Campus, Khandwa Road, Indore-452001, India — [2]Max-Planck-Institut für Festkörperforschung, Heisenbergstr. 1, D-70569 Stuttgart, Germany

We have successfully grown defect free ultra-high quality single crystals of Cr doped Ta2NiSe5, maximum of 10% at Ni site in the lattice. Our preliminary STM results unambiguous provide clear signature of CDW phase, vdW layers and the vdW gap for Ta2NiSe5 which was found to be ~3.5 Å. We found a clear anomaly at the critical temperature Tc = 326 K in our transport measurement over rod shaped crystals - a transition into an excitonic insulator ground state as reported for parent Ta2NiSe5 compound. It is noteworthy to highlight our finding that Cr doping significantly suppresses the insulating ground state and the 10% doping reduces the resistivity of three orders. In addition, our detailed high-temperature Raman scattering for parent as well as Cr doping reveals sharp Raman modes and significant shift and suppression for 230 cm-1 phonon mode which might be associated with electron-phonon coupling, which may helps in resistivity drop as evident in our transport data. In addition, our detailed Raman scattering study suggests the persistence of lattice softening which may be due to strong electron-lattice coupling, and the origin is presumably due to strong excitonic fluctuations.

MM 6.10 Mon 18:15 H10

Magnetic Imaging of the Local Insulator to Metal Transition in CaRuO by NV Magnetometry — •Hayden Binger[1], Cissy Suen[2], Elina Zhakina[1], Luke Turnbull[1], Yejin Lee[1], Young-Gwan Choi[1], Max Krautloher[2], Bernard Keimer[2], Claire Donnelly[1], and Uri Vool[1] — [1]Max Planck Institute for the Chemical Physics of Solids,Dresden, Germany — [2]Max Planck Institute for Solid State Research, Stuttgart, Germany

The current-driven insulator to metal transition in $Ca_2Ru_2O_4$ is a fascinating phenomenon where increasing current driven across a sample causes a smaller voltage difference to develop. While this transition has been well studied in bulk $Ca_2Ru_2O_4$ through transport, and recently investigated by ARPES, little is known about the local character of the transition - especially in nanoscale devices. In this work we utilize scanning NV magnetometry to measure the local magnetic field induced by the local current in 100 nm thick lamellas of $Ca_2Ru_2O_4$. We observe a nonuniform field distribution that reveals the local current channels, allowing us to image the local character of the insulator to metal transition in $Ca_2Ru_2O_4$.

MM 7: Materials for the Storage and Conversion of Energy

Hydrogen related Surface Effects

Time: Monday 15:45–17:00 Location: H22

MM 7.1 Mon 15:45 H22

Effect of stress induced nanohydride formation on dislocation nucleation and pinning in FeCr alloys — •Ali Tehranchi[1], Jing Rao[2], Lekshmi Sreekala[2], Jazmin Duarte[2], Gerhard Dehm[2], Jörg Neugebauer[2], and Tilmann Hickel[1] — [1]BAM Federal Institute for Materials Research and Testing, ali.tehranchi@bam.de, Germany — [2]Max Planck Institute for Sustainable Materials

The detrimental effects of hydrogen (H) on the mechanical properties of metals are universally acknowledged. However, the mechanisms behind these effects remain unclear. In situ nano-indentation experiments are powerful tools for probing the effect of H on the hardness and plasticity of metals. In this work, ab initio calculations and stress dependent phase diagrams in chemical potential space are used to clarify the effect of nanohydrides on the pop-in load of in situ nanoindentation of FeCr alloys. It is shown that the anisotropic stress field of the indenter with a radius of 170 nm facilitates the formation of nanohydrides with significantly lower elastic constants and containing high eigen shear strain. The shear stress associated with these inhomogeneous inclusions is responsible for the experimentally observed reduction in critical shear for dislocation nucleation and the pop-in loads in these indentation experiments. On the other hand, for indenters with a larger radius, the pop-in load is increased due to the pinning of the pre-existing dislocations by the same nanohydrides which are not capable to form underneath the indenter because of the lower magnitude of its induced stress field. The formation of nanohydrides under loading has significant implications for H-embrittlement and H-storage.

MM 7.2 Mon 16:00 H22

Spherical nanoindentation during electro chemical nanoindentation — •Verena Maier-Kiener, Stefan Zeiler, and Anna Jelinek — Montanuniversität Leoben, Leoben, Österreich

Nanoindentation enables efficient characterization of material flow behavior, offering reliable results with minimal effort. While established for hardness and Young*s modulus, its potential for deriving localized flow curves remains underexplored due to challenges in correlating spherical indentation and uniaxial data. A calibration procedure addressing tip imperfections allows strain-rate-controlled experiments and accurate constraint factor evaluation. Using an innovative in-situ electrochemical charging method, side-charging cell, it is shown that electrochemical charging increases hardness and flow stress while reducing the constraint factor, providing valuable insights into deformation behavior.

MM 7.3 Mon 16:15 H22

Hydrogen-based reduction of iron oxide surfaces studied by ab-initio calculations — •Ahmed Abdelkawy, Mira Todorova, and Jörg Neugebauer — Max Planck Institute for Sustainable Materials, Max-Planck-Str.1, 40470 Düsseldorf

The production of pure iron from the iron oxide ores is a very energy-intensive process. Additionally, the dependency on carbon and carbon monoxide as reducing agents results in CO2 as an intrinsic byproduct of the reaction. Consequently, the steel industry is responsible for more than 6% of the global CO2 emissions. Using Hydrogen (H) as a reducing agent would result in water being released instead. Two important aspects in this context are (i) the relative thermodynamics stability of iron oxide facets under different conditions, as this will determine their abundance and (ii) the interaction of H with the oxide surfaces, as these will catalyse the reaction. This work, which is an initial step toward understanding the complex process of the H-based reduction of iron oxides, focuses on Hematite (Fe2O3). Using density functional theory (DFT) calculations we explore the surface stability of different facets under relevant thermodynamic conditions. Additionally, we use transition state theory to describe different H reaction paths and their activation barriers. Keeping in mind the impact the description of the electronic structure may have on the considered quantities, the calculations were performed using both GGA-PBE and GGA-PBE+U. While our results indicate that both methods result in the same preferential reaction path, the electron localization from the (+U) term results in a significant reduction in the activation barrier.

MM 7.4 Mon 16:30 H22

Atomic Cluster Expansion potential for hydrogen-based direct reduction of iron oxides — •Baptiste Bienvenu[1], Mira Todorova[1], Jörg Neugebauer[1], Matous Mrovec[2], Yury Lysogorskiy[2], Ralf Drautz[2], and Dierk Raabe[1] — [1]Max Planck Insitute for Sustainable Materials, Max-Planck-Straße 1, 40237 Düsseldorf, Germany — [2]Interdisciplinary Centre for Advanced Materials Simulation, Ruhr Universität Bochum, 44780 Bochum, Germany

Modeling atomistic mechanisms underlying hydrogen-based direct reduction of iron oxides poses many great challenges, due to the combined structural and electronic complexities of the bulk materials, but also due to the involved chemical reactions. To allow for atomic scale modeling of such processes over the relevant length and time scales, an accurate yet affordable interatomic potential is needed.

Following our previous work, which focused on the development of an Atomic Cluster Expansion (ACE) potential for iron and its oxides, we present in this work the extension of the model to include hydrogen. Based on an extensive DFT-computed database encompassing both iron and its oxides in a wide range of atomic environments involving hydrogen, we fit the extended ACE potential, also including magnetic degrees of freedom. To demonstrate the capabilities of the ACE potential, we focus on its ability to capture some basic mechanisms involved in the hydrogen-based reduction of iron oxides in various environments, including iron oxides-hydrogen (reactions at surfaces, bulk defects), iron oxides-water (surface oxidation), iron-water (surface reactions) and iron-hydrogen (trapping, interactions with defects).

MM 7.5 Mon 16:45 H22

Investigating phase diagram and phonons in superconducting Lanthanum Hydride through an accurate treatment of anharmonicity and nuclear quantum effects — •Abhishek Raghav[1], Kousuke Nakano[2], and Michele Casula[1] — [1]Institut de Minéralogie, de Physique des Matériaux et de Cosmochimie (IMPMC), Sorbonne Université, Paris, France — [2]Center for Basic Research on Materials, National Institute for Materials Science (NIMS), Tsukuba, Japan

Hydrogen rich materials with clathrate structures are an important class of superconducting materials. Lanthanum hydride (LaH_{10}) is one such material, demonstrated to show superconductivity at 250 K and 170 GPa. Phase diagram, phonon spectrum and electron-phonon coupling are important ingredients used to predict superconductivity, being of BCS type. However, computing these accurately for hydrogen clathrate materials requires including anharmonicity due to nuclear quantum effects (NQE). In this work, we use the path integral molecular dynamics (PIMD) and the stochastic self-consistent harmonic approximation (SSCHA) to study NQE and finite temperature on the phase stability and phonons. In order to speed up PIMD and SSCHA calculations, we employ a machine learning potential generated using MACE. This allows us to explore the theoretical LaH$_{10}$ phase diagram over an unprecedentedly wide range of temperatures and pressures. We found that, when quantum effects are included, hydrogen cage symmetrization occurs at lower pressures than in classical simulations, placing the maximum of T$_c$ measured in experiments close to the quantum transition region.

MM 8: Materials for the Storage and Conversion of Energy (joint session MM/KFM)

Lithium-based Materials

Time: Monday 17:15–18:30 Location: H22

MM 8.1 Mon 17:15 H22

Lithium diffusion pathways in modern solid state Li conductors — •Mykhaylo Monchak[1], Volodymyr Baran[2], Stefan Strangmüller[3], and Anatoliy Senyshyn[3] — [1]Institut für Angewandte Materialien, Karlsruhe Institute of Technology, 76344 Eggenstein-Leopoldshafen, Germany — [2]Deutsches Elektronen Synchrotron, 22607 Hamburg, Germany — [3]Heinz Maier-Leibnitz Zentrum, Technical University of Munich, 85748 Garching, Germany

The rapid development of energy storage demands cheaper, more robust electrode and electrolyte materials with improved electrochemical performance. Energy storage and conversion primarily rely on diffusion-based processes, making understanding diffusion pathways crucial. However, determining diffusion pathways in polycrystalline (non-cubic) materials is challenging using bulk or local measurements. Theoretical approaches like molecular dynamics simulations face numerous computational limitations. Alternatively, diffusion processes can be predicted from crystal structures using scattering density maps (electron for X-ray or nuclear for neutrons). These maps analyzed via probability density functions or reconstructed through the maximum entropy method (MEM) are highly reliable. MEM is particularly effective for powder-averaged diffraction data, detecting weak structural disorders. This study applies high-resolution neutron powder diffraction and MEM analysis to explore state-of-the-art lithium conductors considered for application in all-solid-state Li-ion batteries, providing insights into their diffusion pathways and systematics.

MM 8.2 Mon 17:30 H22

"Effortless Embedding": Non-Parametric Solid-State Embedding for NMR Computations using All-Electron DFT — •Federico Civaia[1], Simone S. Köcher[2,1], Karsten Reuter[1], and Christoph Scheurer[1,2] — [1]Fritz-Haber-Institut der MPG, Berlin — [2]Institute of Energy Technologies (IET-1), Forschungszentrum Jülich GmbH, Jülich

Solid-state electrolytes are crucial in lithium-ion battery research, because of the pressing need for safe and durable high-energy storage solutions. Understanding Li-ion dynamics in these materials is essential for developing improved battery technologies. Owing to its non-destructive nature and sensitivity to atomic environments, solid-state nuclear magnetic resonance (SS-NMR) spectroscopy has become an invaluable tool for probing diverse Li-ion environments and investigating Li-ion mobility.

To facilitate the interpretation of experimental Li SS-NMR spectra, we are developing a method for computing NMR parameters of diamagnetic Li compounds using the linear-scaling, all-electron, density functional theory code FermiONs++ [1]. To allow the description of both crystalline and disordered materials, we employ a SS embedding method. In this regard, we present a consistent, non-parametric hybrid Quantum Mechanics/Molecular Mechanics (QM/MM) methodology for systematic and reproducible structure generation and SS embedding calculations.

[1] J. Kussman *et al.*, J. Chem. Phys. **138**, 134114 (2013); J. Chem. Theory Comput. **11**, 918 (2015).

MM 8.3 Mon 17:45 H22

Insights into Li-ion battery cathode redox chemistry via charge transfer multiplet simulations of LiNi$_{1/3}$Mn$_{1/3}$Co$_{1/3}$O$_2$ — •Ruiwen Xie[1], Maximilian Mellin[2], Wolfram Jaegermann[2], Jan. P Hofmann[2], and Hongbin Zhang[1] — [1]Theory of Magnetic Materials Group, Department of Materials and Geosciences, Technical University of Darmstadt — [2]Surface Science Laboratory, Department of Materials and Geosciences, Technical University of Darmstadt

The evolution of electronic structure during discharging and charging processes with Li intercalation and deintercalation in transition metal oxide cathode materials involves changes in oxidation states, non-rigid band behavior, and oxygen's role in charge compensation, which significantly impact cathode performance. To gain deeper insights, we combine experimental x-ray photoelectron spectroscopy (XPS) at various voltages with many-body electronic structure simulations. The electronic structures of Li$_x$CoO$_2$ and Li$_x$NiO$_2$ were calculated using Density Functional Theory and Dynamical Mean-Field Theory (DFT+DMFT). We found that Li intercalation and deintercalation shift the hybridization between Co/Ni d and O p orbitals relative to the Fermi energy, altering Co/Ni d occupancy. Based on this, we performed XPS calculations using the multiplet ligand-field model in Quanty to revisit the transition metal 2p satellite structure evolution. This study provides crucial insights into the interplay between electronic structure and Li intercalation dynamics for enhancing cathode performance.

MM 8.4 Mon 18:00 H22

Modelling LLZO Grain Boundaries with Amorphous Domains by Adaptively Trained Machine-Learning Interatomic Potentials — •Yuandong Wang, Yute Chan, Hao Wan, Kyeonghyeon Nam, Karsten Reuter, and Christoph Scheurer — Fritz-Haber-Institut der MPG, Berlin

Garnet Li$_7$La$_3$Zr$_2$O$_{12}$ (LLZO) is a highly promising solid state electrolyte (SSE) for lithium batteries. However, its practical application faces challenges, primarily arising from Li dendrite formation and the impact of grain boundaries (GBs) on Li transport and stability. Amorphous LLZO combines several desirable properties like blocking Li dendrite growth, high Li mobility and high electronic impedance. Controlling amorphous domains between crystalline grains could therefore offer an intriguing approach to tune electrolyte performance. For this, an atomistic understanding of the interplay between composition, structure and the properties of LLZO glass-ceramics is crucial.

This study introduces a Machine Learning Interatomic Potential (MLIP) tailored to accurately represent amorphous and GB structures in LLZO. Developed through an iterative training protocol using simulated annealing, this MLIP includes diverse structures in its training set, ensuring comprehensive modeling of complex LLZO phases. The MLIP enables large-scale molecular dynamics simulations, allowing the construction of realistic amorphous and GB models, and providing a foundation for in-depth analysis of LLZO structural and electrochemical behavior.

MM 8.5 Mon 18:15 H22

Early Stage of Li Cluster Nucleation at the Li Anode-Solid Electrolyte Interface in Solid-State Batteries — •Yun An[1,2], Taiping Hu[2], Quanquan Pang[2], and Shenzhen Xu[2] — [1]Fritz-Haber- Institut der MPG, Berlin, Germany — [2]School of Materials Science and Engineering, Peking University, Beijing, China

Li dendrite formation inside all-solid-state lithium batteries (ASSBs) strongly impedes their practical applications. Despite this recognized challenge, a comprehensive understanding of the Li dendrite nucleation mechanism remains elusive. In particular, the initial sites of Li dendrite formation are still ambiguous: do Li clusters form directly at the Li anode surface, or do they nucleate at a distance from the Li metal surface?

Here, based on deep-potential molecular dynamics simulations combined with enhanced sampling techniques, we investigate the atomic-level mechanism of Li cluster nucleation sites in ASSBs. We observe isolated Li clusters initially forming inside the solid electrolyte interphase (SEI), located approximately 1 nm away from the Li anode/SEI boundary, rather than directly connected to the Li anode. The local electronic structure of the spontaneously formed SEI is a key factor enabling the Li cluster formation within SEI. Our work provides atomic-level insights into initial Li-dendrite nucleation sites in ASSBs and could guide future design for developing Li-dendrite-inhibiting strategies.

MM 9: Poster

Time: Monday 18:30–20:30 Location: P1

MM 9.1 Mon 18:30 P1

Well-defined nanostructures synthesized by optimized anodic aluminum oxide template — •Linfeng Su, Huaping Zhao, and Yong Lei — Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany

The template method has unique advantages in the design and synthesis of materials with specific nanostructures but with some disadvantages. In recent years, through in-depth research and improvement of its preparation methods, the five shortcomings of the traditional anodic aluminum oxide (AAO) template method, such as short-range order and long-range disorder, insulator, single-set of pores, large dead volume, and limited capability to tune pore shape and arrangement, have been successfully addressed by our group. Large-scale control of the shape, size, spatial configuration, and combination of in-plane and out-of-plane pores of well-defined nanostructures can be achieved, thereby broadening the diversity of nanostructures[1, 2]. In addition, we have improved the mechanical strength of the prepared AAO template, so that it can maintain the stability of the nanostructure under a pressure of 10 MPa[3]. The optimized AAO template method provides practical guidance for the design and preparation of catalysts under complex application conditions. [1] Nat. Commun., 2022, 13(1), 2435; [2] Nat. Nanotechnol., 2017, 12(3), 244; [3] Nat. Commun., 2020, 11(1), 299.

MM 9.2 Mon 18:30 P1

Ferroelectric perovskite oxides: PFM investigations of (001) surface — •Andrzej Jasicki[1], Marta Macyk[1], Llorenç Albons[2], Konrad Szajna[1], Martin Setvin[2], Dominik Wrana[1], and Franciszek Krok[1] — [1]Marian Smoluchowski Institute of Physics, Jagiellonian University, Krakow, Poland — [2]Department of Surface and Plasma Science, Charles University, Prague, Czech Republic

Growing demand for energy from green sources drives development in this sector. Hydrogen, as one of the most promising fuels, is mostly produced with the use of electricity during electrolysis, what lowers the overall efficiency of whole process. To reduce energy costs, one should search for an efficient water-splitting catalyst.

Although ferroelectric perovskite oxides show great potential in photocatalysis, it can be further enhanced via piezo- and pyrocatalysis. In order to understand their role in water-splitting process, a thorough investigation of ferroelectricity manifested at surfaces is necessary. Piezoresponse Force Microscopy (PFM), a method based on inverse piezoelectric effect, provides an opportunity to have a closer look into surface domain structure of such materials.

This poster displays PFM and SEM data obtained by investigations into domain structure on surfaces of single-crystalline, ferroelectric perovskites, namely KNbO3 and BaTiO3. Measurements on both polished and cleaved (001) surfaces were conducted in room temperature and under ambient atmosphere. Influence of different poling voltages and exposure to water is also discussed.

MM 9.3 Mon 18:30 P1

Pressure-induced hybridization changes in elemental silicon at Mbar pressure — Robin Sakrowski[1], Christoph J. Sahle[2], •Gordon Scholz[1], Leonie Tipp[3], Mirco Wahab[3], Sindy Fuhrmann[3], and Christian Sternmann[1] — [1]Fakultät Physik / DELTA, Technische Universität Dortmund, Maria-Goeppert-Mayer-Straße 2, 44221, Dortmund, Germany — [2]ESRF, The European Synchrotron, 71 Avenue des Martyrs, CS40220, 38043 Grenoble Cedex 9, France — [3]Institut für Glas und Glastechnologie, TU Bergakademie Freiberg, Leipziger Straße 28, 09599, Freiberg, Germany

Silicon, a fundamental semiconductor material, undergoes intriguing structural and electronic transformations when subjected to high pressure [1]. These changes are investigated using X-ray Raman scattering (XRS) spectroscopy on pure Si powder loaded into a diamond anvil cell for pressures up to 108 GPa. The XRS spectra of the Si $L_{2,3}$-edge are compared with ab-initio theoretical calculations based on the Bethe-Salpeter equation. Observations include an increase in coordination number from 4-fold to 12-fold and metallization. Additionally, changes in the occupation probability of d-states under pressure are noted, as silicon valence electrons from the 3s and 3p orbitals are transferred.

This work is supported by the BMBF projects 05K22PE2 and 05K22OF1. [1] J.S.Tse et al., J. Phys. Chem. C 118, 1161 (2014)

MM 9.4 Mon 18:30 P1

THz signatures of displacive phase transformation — •Nandita Bajpai[1], Michael Dittler[1], Ahana Bhattacharya[1], Alexander Kunzmann[2], Gabi Schierning[2], and Martin Mittendorff[1] — [1]Department of Physics , University of Duisburg — [2]Institute for energy and material process, University of Duisburg

Phase Change Materials are widely applied in contemporary technological advancements such as sensors, activators, and electronic devices. The Terahertz time-domain spectroscopy (THz-TDS) reflectivity and transmissivity measurements provide valuable insights into carrier dynamics such as mobility and carrier concentration. The temperature-induced phase change results in significant changes in reflectivity and transmissivity that are linked to the presence of free electrons.

Furthermore, the change in the complex conductivity points towards the predicted formation of a charge density wave (CDW) phase, which is a manifestation of periodic modulation of the electron density. This provides more details toward understanding the role of electrons in the phase transformation.

MM 9.5 Mon 18:30 P1

Impact of hyperthermal oxygen on alumina surfaces investigated by molecular dynamics simulations — •Stephen Hocker, Hansjörg Lipp, and Johannes Roth — Institut für Funktionelle Materie und Quantentechnologien, Universität Stuttgart

Oxygen atoms impinging on satellite surfaces in very low earth orbit (VLEO) transfer momentum and energy leading to material degradation as well as drag forces which result in orbital decay of the satellite. The first step in finding solutions to counteract significant drag is to gain understanding of the interaction of atomic oxygen (AO) with material surfaces. We investigate the adsorption rate and the angular distribution of reflected AO on crystalline and amorphous alumina surfaces using molecular dynamics simulations. It is found that the angular distribution depends strongly on the surface structure and the incidence angle. A higher ratio of specular reflection is found in case of smooth surfaces and large incidence angles.

MM 9.6 Mon 18:30 P1

Ultrafast phonon-mediated dephasing of color centers in hexagonal boron nitride probed by electron beams — •Masoud Taleb[1], Mario Hentschel[3], Harald Giessen[3], and Nahid Talebi[1,2] — [1]Institute of Experimental and Applied Physics, Kiel University, 24098 Kiel, Germany — [2]Kiel Nano, Surface and Interface Science KiNSIS, Kiel University, 24118 Kiel, Germany — [3]4th Physics Institute and Research Center SCoPE, University of Stuttgart, 70569 Stuttgart, Germany

Defect centers in hexagonal boron nitride (hBN) have gained significant interest as room-temperature single-photon sources, with strong coupling to phonons evident in their photoluminescence and cathodoluminescence spectra. Despite extensive studies, the electron-phonon coupling dynamics and phonon-mediated dephasing of these centers remain underexplored. In this study we experimentally employed an electron-driven photon source (EDPHS) to generate a coherent superposition of phonon states, with the delay between electron and photon pulses controlled to measure dephasing times. The findings reveal an ultrafast dephasing time of 200 fs and a radiative decay of 585 fs at room temperature, contradicting other optical techniques reporting a decay of a few nanoseconds. This rapid dephasing is attributed to the efficient excitation of coherent phonon-polaritons in hBN by electron beams. The research demonstrates the capability of sequential CL spectroscopy for probing the ultrafast dynamics of single emitters in quantum materials, facilitating future applications in quantum networks and devices.

MM 9.7 Mon 18:30 P1

Raman spectroscopic studies on $NiFe_2O_4$-NiO-Ni and MgO-Steel composites as inert anode materials for aluminium molten salt electrolysis — •Felix Drechsler[1], Ulziikhuu Otgonbayar[2], Cameliu Himcinschi[1], and Jens Kortus[1] — [1]TU Bergakademie Freiberg, Institute of Theoretical Physics, D-09599 Freiberg, Germany — [2]TU Bergakademie Freiberg, Institute of Nonferrous Metallurgy and Purest Materials, D-09599 Freiberg, Germany

The use of inert anodes in aluminium molten salt electrolysis offers positive environmental effects compared to the commercially used graphite anode, especially by avoiding CO, CO_2 and perfluorocarbon (PFC) emissions. Cermet anodes consisting of $NiFe_2O_4$, NiO, and Ni were manufactured by powder metallurgy and sintered at different conditions using the Spark Plasma Sintering (SPS) technique. Furthermore, another type of anode was produced using MgO and steel powder mixture to form metalloceramic composites. These anode materials were investigated by micro-Raman spectroscopy to identify phases formed during the sintering process, such as nickel ferrite spinels. Temperature-dependent Raman measurements were performed to examine the micro-structure behaviour of the anode materials at elevated temperatures.

MM 9.8 Mon 18:30 P1

Influence of the alloying elements on microchemistry and nanostructure of Sm-Co based permanent magnets — •Burçak Ekitli[1], Alex Aubert[1], Fernando Maccari[1], Nikita Polin[2], Xinren Chen[2], Esmaeil Adabifiroozjaei[3], Leopoldo Molina-Luna[3], Baptiste Gault[2], Konstantin Skokov[1], and Oliver Gutfleisch[1] — [1]Functional Materials, TU Darmstadt, 64287 Darmstadt, Germany — [2]Max-Planck-Institut for Sustainable Materials, Düsseldorf 40237, Germany — [3]Advanced Electron Microscopy, TU Darmstadt, 64287 Darmstadt, Germany

Sm-Co 2:17 magnets are high-temperature, high-performance magnets that are commercially available. Their hard magnetic properties are driven by a pinning mechanism, where the complex microstructure and microchemistry play an important role [1]. Since commercial 2:17 magnets consist of five alloying elements and three coherent phases, it is difficult to establish a common understanding of their intrinsic and extrinsic properties. In this study, we continue to investigate the 2:17 magnet system, focusing on a simplified alloy system that we initially introduced [2] by adding Cu to the alloy. Our study focuses on the quaternary Sm(Co,Cu,Zr)6.7 alloy, with four different compositions chosen based on varying Cu concentrations. We investigate the microstructural properties and their influence on the hysteresis of the Sm-Co 2:17 magnet in detail, using advanced characterization techniques such as MOKE, MFM, TEM, and APT. We reveal how Cu concentration influences the microstructure and phase formation, ultimately affecting the magnetic properties.

MM 9.9 Mon 18:30 P1

Bonding changes in solid nitrogen under high pressure — Gordon Scholz[1], Robin Sakrowski[1], Johannes Niskanen[2], Christoph Sahle[3], Leonie Tipp[4], Mirco Wahab[4], Melanie White[5], •Peter Schäfer[1], Ashkan Salamat[5], Sindy Fuhrmann[4], and Christian Sternemann[1] — [1]TU Dortmund, Dortmund, Germany — [2]University of Turku, Turku, Finland — [3]ESRF, Grenoble, France — [4]TU Bergakademie Freiberg, Freiberg, Germany — [5]University of Nevada Las Vegas, Las Vegas, USA

Nitrogen has a complex phase diagram with 15 detected solid molecular phases [1]. In this study, we tracked the electronic and structural changes of nitrogen under high pressure using a novel combined set-up for X-ray Raman scattering (XRS) and X-ray diffraction (XRD) at beamline ID20 at the ESRF exploiting the diamond anvil cell method.

In the pressure regime between ambient conditions and 80 GPa we are able to confirm the δ-phase, ϵ-phase and the ζ-phase with XRD. The corresponding XRS measurements at the nitrogen K-edge show significant changes in the bonding structure. These changes are interpreted via calculated XRS spectra based on molecular dynamic simulations which reveal a hindrance of free rotations of the N_2 molecules in the ϵ-phase.

This work is supported by the BMBF via the projects 05K22PE2 and 05K22OF1.

[1] Turnbull et al. Nat. Commun., 9:4717, (2018)

MM 9.10 Mon 18:30 P1

Grain boundary transformation induced by boron segregation — Xuyang Zhou[1], •Sourabh Kumar[2], Siyuan Zhang[1], Xinren Chen[1], Baptiste Gault[1], Gerhard Dehm[1], Tilmann Hickel[1,2], and Dierk Raabe[1] — [1]Max-Planck-Institut für Eisenforschung, Düsseldorf, 40237, Germany — [2]Bundesanstalt für Materialforschung und -prüfung (BAM), Berlin, 12489, Germany

The segregation of solute atoms at grain boundaries (GBs) critically influences the mechanical properties of materials, including corrosion resistance and fracture toughness. This study examines structural transformations induced by minimal boron concentrations at $\Sigma 13$ GBs in ferrite thin films. Two sample protocols were investigated: one with carbon as the sole solute and the other with carbon and boron co-segregation. Using ab initio calculations, we meticulously explored the competing $\Sigma 13$ GB phases coexisting with defects and analyzed the energetics of solute segregation at the GB interface. A defect phase diagram was constructed to illustrate the influence of B concentration on GB structure evolution. We reveal that B segregation transforms the GB structure from flat to zigzag trigonal prisms by forming new chemical bonds, enhancing B-Fe bonding strength by 5%. This transformation doubles steel's fracture resistance and provides valuable insights into solute-driven GB phase evolution, contributing to innovative strategies for designing durable, high-performance steel.

MM 9.11 Mon 18:30 P1

Investigation of spin-crossover iron triazole complexes with carbon nanotubes — •Niloofar Azadegan[1], Marvin Dzinnik[2], Maximilian Kilic[3], Franz Renz[4], and Rolf Haug[5] — [1]Institute of solid state physics, Hannover, Germany — [2]Institute of solid state physics, Hannover, Germany — [3]Institute of inorganic chemistry, Hannover, Germany — [4]Institute of inorganic chemistry, Hannover, Germany — [5]Institute of solid state physics, Hannover, Germany

Iron triazole complexes exhibit spin-crossover (SCO) behavior, transitioning between low-spin and high-spin states under external stimuli, making them suitable for sensing and memory applications.

This study investigates carbon nanotubes (CNTs) decorated with iron triazole to enhance electronic and magnetic properties. Current-voltage measurements were performed on bare and decorated CNTs, followed by cryostat measurements under controlled conditions. Preliminary results suggest interactions between SCO behavior and CNTs, with ongoing analysis to explore their potential in advanced electronics.

MM 9.12 Mon 18:30 P1

Linking Characteristic Length Scale in Nanoporous Gold to Alloy Composition and Dealloying Parameters — •Celina Passig[1,2], Jürgen Markmann[2,1], and Jörg Weissmüller[1,2] — [1]Institute of Materials Physics and Technology, Hamburg University of Technology, Germany — [2]Hybrid Materials Systems, Institute of Hydrogen Technology, Helmholtz-Zentrum Hereon, Geesthacht, Germany

Nanoporous metals display unique material properties due to their high volume-specific surface area and characteristic sizes of pores and ligaments. Although theories of structure formation exist, the process is not yet fully understood. Investigating nanoporous gold as model system will deepen the understanding of the underlying mechanisms, enabling a more precise manipulation of nanoporous structures and their mechanical and functional properties. Therefore, a series of small-angle X-ray scattering (SAXS) data was measured, comparing AuAg alloy compositions subjected to different dealloying potentials, durations, and electrolyte concentrations. Preliminary dependencies were formulated to investigate how these parameters influence the resulting characteristic length scale. This ex-situ and future in-situ analysis of microstructural evolution can be used to identify the underlying mechanisms by validating simulated results of the same dealloying processes, such as those presented by Li et al. [Acta Mater. 222 (2022) 117424.].

MM 9.13 Mon 18:30 P1

Inhomogeneities at different length scales in nanocrystalline Pd-Au prepared by inert gas condensation — Johannes Wild[1], Fabian Andorfer[4], Svetlana Korneychuk[1,2,3], Jules M. Dake[4], Torben Boll[1], Dorothée Vinga Szabó[1,2,3], Stefan Wagner[1], Carl E. Krill III[4], and •Astrid Pundt[1,2] — [1]Institute of Applied Materials (IAM-WK), Karlsruhe Institute of Technology —

[2]Institute of Nanotechnology (INT), Karlsruhe Institute of Technology — [3]Karlsruhe Nano Micro Facility (KNMFi), Karlsruhe Institute of Technology — [4]Institute of Functional Nanosystems, Ulm University

Inert gas condensation (IGC) is currently the only viable method to prepare bulk samples of nanocrystalline (NC) palladium-gold (Pd-Au). The raw material is thermally evaporated in a vacuum chamber with a background pressure of 10e-8 mbar that has been backfilled with low-pressure inert gas. On collision with the inert gas, the evaporated material condenses into small particles, which are then collected on a rotating cold finger, scraped off and mechanically compacted into disk-shaped samples.

In this study, we investigate the different types of inhomogeneities in IGC Pd-Au on different length scales and compare them to samples prepared by arc melting. To this end, we apply a variety of methods to accurately characterize the composition, porosity, grain size, grain orientation and grain growth behaviour on multiple length scales. Finally, we attempt to explain the source of the inhomogeneities and verify by probing the IGC experimental setup via various experiments.

MM 9.14 Mon 18:30 P1

Development, Characterization and Catalytic Evaluation of New Nanosized metal complexes — •Tarek El-Dabea — Chemistry Department, Faculty of Science, King Salman International University, Ras Sudr, Sinai 46612, Egypt

A series of novel nano metal complexes involving Pd(II), Cu(II), Fe(III) and Ag(I) ions were synthesized using a Schiff base ligand in a bidentate coordination mode. The structural and molecular characteristics of these complexes were thoroughly characterized via an array of spectroscopic and analytical techniques, confirming molecular geometry and stoichiometry. Solution stability and stoichiometry of the complexes were systematically evaluated, demonstrating stable metal-ligand coordination. Notably, the Pd(II) complex exhibited unique electronic characteristics, identifying it as a promising candidate for catalytic applications. Based on these results, the Pd(II) complex was tested as a catalyst for synthesizing Different multicomponent reactions. This was achieved through using microwave irradiation. The selection of Pd(II) was informed by its favorable catalytic profile and theoretical insights. Optimization trials demonstrated that the Pd(II) catalyst afforded high yield and efficiency under eco-friendly (H*O/EtOH) solvent conditions. Reusability assessments showed that the catalyst retained high activity for up to five cycles, with minimal performance decline afterward. A mechanistic pathway was proposed, highlighting Pd(II)'s ability for axial coordination, supported by theoretical evidence

MM 9.15 Mon 18:30 P1

Epitaxial Stabilization of Multifunctional Oxide, Oxynitride, and Telluride Thin Films using a Hybrid Pulsed Laser Deposition Technique — Pia Henning, Anna Tschesche, Shagun Thakur, Niklas Kohlrautz, Abhishek Sharma, Laura Pflügl, and •Jasnamol Palakkal — Institute of Materials Physics, Georg-August-University of Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

Materials science uses state-of-the-art thin film techniques, such as pulsed laser deposition (PLD) and molecular beam epitaxy (MBE), to artificially fabricate complex materials [1]. Epitaxial films with controlled defects and orientation are practical for modifying functionalities. We developed a hybrid PLD system attaching molecular beam sources (for elements with high vapor pressure) to fabricate multifunctional oxide, oxynitride, and tellurides. Additionally, gases are provided through a microplasma source. This setup makes a wide range of cation and anion engineering possible in complex materials. In this presentation, we will address challenges in the growth of thin films and how modifications in the defects and structure influence functional properties by taking examples of La$_2$NiMnO$_6$ (ordered magnetism and electrocatalysis), Cr$_x$Te (ferromagnetism and magnetic anisotropy), and SrNbO$_3$ (optical transparency and metallic conduction). Moreover, we will discuss how such a hybrid deposition system can be utilized to grow high-entropy materials and stabilize doping beyond the solubility limit. [1] A. Tschesche, et al., Preprint on Research Square, https://doi.org/10.21203/rs.3.rs-4861088/v1

MM 9.16 Mon 18:30 P1

EXAFS-driven Investigation of ZnO-Mn2O3 and ZnO-Mn2O3-rGO Nanocomposites: Unraveling Structural, Optical, and Electronic Properties — •Shaimaa A. Habib[1], Shehab E. Ali[2], Messaoud Harfouche[3], and Ahmed Awad[4] — [1]1.*Physics Department, Faculty of Science, Damnhour University, Damanhour 22516, Egypt — [2]Materials Science Laboratory, Physics Department, Faculty of Science, Suez Canal University, 41522, Ismailia, Egypt. — [3]SESAME (Synchrotron-light for Experimental Science and Applications in the Middle East), Allan, Jordan — [4]Physics Department, Faculty of Science, Tanta University, Tanta 31527, Egypt

The structural, optical, and electronic properties of ZnO-Mn2O3 and ZnO-Mn2O3-rGO nanocomposites were investigated. The materials, synthesized via sol-gel and self-propagation methods, exhibited porous structures with crystallite sizes of 22-48 nm, as confirmed by XRD and SEM analyses. UV-Vis spectroscopy revealed that rGO incorporation reduced the optical bandgap from 2.63 eV to 1.86 eV and increased the Urbach energy from 1.91 eV to 2.55 eV. The Wemple-DiDomenico model showed a decrease in oscillator resonance energy from 6.64 eV to 6.15 eV and an increase in dispersion energy from 6.47 eV to 13.24 eV. EXAFS and XANES studies at SESAME synchrotron facility provided insights into the coordination environment and electronic structure of the metal centers. This comprehensive characterization establishes a foundation for applying these nanocomposites in optoelectronics, photocatalysis, and energy conversion applications, highlighting rGO's role in enhancing composite performance.

MM 9.17 Mon 18:30 P1

Electrochemical determination of the diffusion coefficient of intercalating species in host metals - conditions of applicability of potential step chronoamperometry — •Magdalena Seiler, Giorgia Guardi, Stefan Wagner, and Astrid Pundt — KIT, Karlsruhe, Deutschland

The diffusion coefficient is generally used to describe the diffusion of intercalating species such as lithium and hydrogen in host metals. It can be determined by a variety of methods, including electrochemical methods. Among these, permeation methods between front and back side of a sample are widely used. On the contrary, in potential step chronoamperometry only one side of the sample needs to be contacted, which is e.g. beneficial for thin film studies. In this work measurements using both methods are performed for hydrogen in palladium and compared to the literature. It is shown that the application of the potential step chronoamperometry approach gives correct results only under very specific restrictions regarding sample thickness and measurement period.

MM 9.18 Mon 18:30 P1

Synthesis, and Characterization of Li/Mn-Excess Cathode Materials for Li-ion Batteries. — •John Karuga[1], Mesfin Kebede[2], and Guido Schmitz[3] — [1]Institute of Materials Science, Department for Material Physics, University of Stuttgart — [2]Institute of Nanotechnology and Water Sustainability, College of Science, Engineering and Technology, University of South Africa — [3]Institute of Materials Science, Department for Material Physics, University of Stuttgart

The study aims to mitigate O2 evolution, spinel phase, and unstable CEI formation common in Li/Mn-excess cathodes. The poster presents preliminary results of the pristine Li/Mn-excess cathodes, which are practical alternatives to LFP, NCA, and Ni-excess materials for high-performance Li-ion batteries. The Li2MnO3 phase in Li/Mn-excess cathodes stabilizes the crystal structure, contributes to the higher discharge capacities >250 mAh/g. Commercialization of Li/Mn-excess materials remains challenging due to undesired transformation from layered to spinel phase, O2 evolution, parasitic reactions with the LiPF6 electrolyte. The Li/Mn excess materials were prepared via solid-state synthesis. Characterization with SEM-EDS, Raman, HR-TEM, and XRD confirmed the development of a material of uniform nanocrystallites with well-layered structure and 0.472 and 0.2 nm interplanar distances, which correspond to the 003 and 104 planes. The CV analysis confirms that the redox reactions (Ni2+/Ni4+; Co3+/Co4+; Mn3+/Mn4+/5+/7+) are highly reversible. The charge transfer resistance is low, indicative of better Li+ diffusion and stable CEI.

MM 9.19 Mon 18:30 P1

Magnetic anisotropy and anomalous Nernst effect in cubic Fe4N films — •Karel Knížek[1], Jakub Vít[1], Mariia Pashchenko[1], Petr Levinský[1], Kyo-Hoon Ahn[1], Jaroslav Kohout[2], and Imants Dirba[3] — [1]Institute of Physics, Czech Academy of Sciences, Prague, Czechia — [2]Faculty of Mathematics and Physics, Charles University, Prague, Czechia — [3]Functional Materials, Institute of Materials Science, Technical University of Darmstadt, Germany

Iron nitrides Fe(x)N are commercially important compounds because of their versatile magnetic, electrical, and mechanical properties. We have studied magnetic and transverse thermoelectric properties of Fe(4)N films prepared by magnetic sputtering. The well-known anisotropic magnetoresistance [1] and rectangular magnetization curves for thin oriented films led us to investigate magnetic anisotropy by rotating the sample in external magnetic field and measuring magnetization along the field. The signal is complex, exhibiting harmonics beyond the expected crystal symmetry. Moreover, the magnetic-field history crucially impacts the anisotropy. The results are quite distinct below and above the metamagnetic phase transition near 50K. The results of the magnetic measurements are compared with anomalous Nernst effect experiments and DFT calculations.

[1] M. Tsunoda et al., Applied Physics Express 2, 083001 (2009).

MM 9.20 Mon 18:30 P1

Thermoelectricity in Bi-directionally Strained $CsSnI_3$ Perovskite — •Michele Reticcioli[1], Mariangela Ruggeri[2], Giovanna D'Angelo[2], and Alessandro Stroppa[1] — [1]CNR-SPIN L'Aquila, Italy — [2]Università degli Studi di Messina, Italy

Thermoelectric materials play a pivotal role in energy sustainability, converting waste heat into electricity without moving parts or emissions. Recent advances spotlight metal halide perovskites, such as $CsSnI_3$, as promising candidates for eco-friendly thermoelectric applications due to their low thermal conductivity and high electrical efficiency. In this work, we explore the influence of bidirectional strain on the orthorhombic gamma-phase of $CsSnI_3$ using density functional theory (DFT), complemented by experimental insights from our collaborators. Strain effects, ubiquitous in thin films grown on mismatched substrates, are known to modify electronic structures and transport properties. Our findings reveal a peculiar dependence of the bandgap on strain direction and intensity. These changes directly impact the thermoelectric properties, including the Seebeck coefficient and figure of merit, emphasizing the interplay between strain-induced electronic modulation and thermoelectric performance. This study contributes to the growing understanding of strain effects in perovskites, offering valuable insights into their potential for thermoelectric applications.

MM 9.21 Mon 18:30 P1

GAP vs. MACE: Efficiency evaluation in a liquid electrolyte system — •Anton Beiersdorfer[1], Lisa Hetzel[1], Carsten Staacke[2], Florian Deissenbeck[2], and Christopher Stein[1] — [1]Technische Universität München, München, Germany — [2]Cellforce Group GmbH, Tübingen, Germany

Machine learning interatomic potentials (MLIP) have transformed molecular simulations, enabling complex materials to be modeled with increasing accuracy and efficiency. As MLIP models evolve, so does the demand for advanced computing architectures, particularly graphics processing units (GPUs), which can accelerate computations compared to traditional central processing unit (CPU) based systems. However, the high cost associated with GPU resources constrain access in both academia and industry, highlighting the relevance of comparing GPU-based and CPU-based MLIPs under real-world conditions.

To this end two popular MLIPs are examined: the GPU-accelerated MACE model and the CPU-based GAP model applied to a test system of a standard battery electrolyte. The system is selected for its demanding electrostatic interactions in solution, which the MLIPs approximate by learning the local interaction patterns that contribute to the overall electrostatic behavior. Therefore, it represents a significant computational challenge and provides a rigorous benchmark for MLIP accuracy and efficiency. By focusing on these models, the study aims to reveal key differences in computational and numerical performance metrics and resource efficiency as well as in physical performance, particularly through comparisons to experimentally measured properties.

MM 9.22 Mon 18:30 P1

Navigating the Latent Space of Chemical Solid State Reactions in Hybrid Battery Interfaces — •Sina Ziegler, Christoph Scheurer, and Karsten Reuter — Fritz-Haber-Institut der MPG, Berlin

We explore the potential of rare earth lithium halides as a material-efficient, nanometer-thick cathode coating in contact with thiophosphate electrolytes. Traditional theoretical approaches, such as molecular dynamics (MD) and Monte Carlo (MC) simulations, are computationally intensive for larger systems, posing a challenge in simulating battery interfaces. To identify a suitable halide/thiophosphate combination, it is essential to determine an energetically feasible solid-state reaction pathway within the multidimensional phase diagram of these materials. We employ *ab initio* thermodynamics to assess the thermodynamic stabilities of the resulting solid-state electrolyte (SSE) and halide interfaces by screening the reaction-free enthalpies of potential interface reactions. An end-member analysis is then performed to evaluate possible compositions of interface products and secondary phases, using techniques such as Principal Component Analysis (PCA), t-distributed Stochastic Neighbor Embedding (t-SNE), and autoencoders to identify linked reactions within the chemical latent space.

MM 9.23 Mon 18:30 P1

Structure and transport properties of Li3MCl6 superionic conductors — •Ziyan Zhang[1,2], Peter Müller-Buschbaum[1], and Anatoliy Senyshyn[2] — [1]Chair for Functional Materials,School of Natural Sciences, Technical University of Munich,85748 Garching, Germany — [2]Heinz Maier-Leibnitz Zentrum, Technical University of Munich, 85748 Garching, Germany

Modern society permanently requires more advanced, better performant, safer, and cost-effective energy storage solutions, where the all-solid-state battery (ASSB) concept based on lithium metal is closest to commercialization. Solid electrolytes are a key component of ASSB, defining its lifetime and performance. Halide-based solid electrolytes Li3MCl6 (M = transition metals, rare-earth metals) are emerging as promising materials for all-solid-state batteries due to their high ionic conductivity, electrochemical stability, and compatibility with lithium metal anodes. The current study deals with the systematic characterization of Li3MCl6 solid conductors with M = In, Zr, and Ti transition elements. The focus will be put on the optimization of synthesis routes (between solvent-mediated and mechanochemistry), composition control as well as enhancement of ionic transport. Comprehensive structural characterization, encompassing lab X-ray diffraction (XRD) with Rietveld refinement combined with differential bond-valence estimates of lithium diffusion pathways and differential scanning calorimetry, is performed to reveal the crystallographic details, microstructure, and lithium-ion dynamics.

MM 9.24 Mon 18:30 P1

Processing of non-conductive materials by electroerosion treatment. — •Anton Bespalov — Moscow, Russia

Electroerosion processes process only conductive materials, but it is possible to process non-conductive materials by applying a thin layer of metal to their surface. In this work, based on experiments, the possibility of destruction (processing) of tungsten carbide coated with a layer of 0.01 mm copper with a copper electrode using electric erosion machines is considered. As a result of the experiments, the destruction in the samples corresponding to the shape of the electrode was revealed, which proves the possibility of processing.

MM 9.25 Mon 18:30 P1

Structure formation and phase behavior of amine-water mixtures — •Lena Friedrich[1], Michael Paulus[1], Aurélien Perera[2], Martina Požar[3], Dirk Lützenkirchen-Hecht[4], Nicola Thiering[1], Jaqueline Savelkouls[1], and Christian Sternemann[1] — [1]Fakultät Physik / DELTA, Technische Universität, 44221 Dortmund, Germany — [2]Sorbonne Université, Laboratoire de Physique Théorique de la Matière Condensée, F75252, Paris cedex 05, France; — [3]University of Split, Faculty of Science, 21000 Split, Croatia — [4]Fakultät für Mathematik und Naturwissenschaften, Bergische Universität Wuppertal, 42097 Wuppertal, Germany

Amines are associating liquids that can form transient supramolecular structures via hydrogen bonding [1]. Adding of water can significantly alter the liquids' structure [2] and amine/water mixtures show an interesting phase behavior exhibiting a lower critical solution temperature (LCST) [3]. We studied linear, primary amines mixed with various proportions of water for a variety of temperatures by X-ray diffraction at BL8 and BL9 of DELTA (TU Dortmund). The structure factor prepeak shows a peculiar concentration and temperature dependence which resembles the different phase regimes ranging from disordered nematic via single liquid to two liquid phase. We thank the BMBF for funding via DAAD in the scope of the French-German collaboration PROCOPE 2024-2025 (Project-IDs 57704875 and 50951YA). [1] A. Perera et al., JPC B 44, 128 (2024). [2] L. Almasy et al., PCCP 21, 9317 (2019); [3] J. Glinski et al., J. Colloid. Interface Sci. 162, 129-134 (1994)

MM 9.26 Mon 18:30 P1

A Phase Change Material's Journey through its Energy Landscape — •Jakob Ballmaier, Sebastian Walfort, Elias Abele, and Martin Salinga — Universität Münster, Institut für Materialphysik

The concept of energy landscapes is highly successful in explaining structural dynamics of supercooled liquids and glasses. Locally stable configurations correspond to local minima of the total potential energy of the system in the high-dimensional phase space. During physical aging a glass can evolve towards lower local minima through a series of saddle points. Experimental observation of this is challenging, since in large systems several saddle points are passed within the shortest resolvable timescales.

Here, we track paths through the energy landscape of a nanoscopic volume of germanium telluride by following the temporal evolution of its electrical resistance. Two regimes turn out to be especially instructive: fast measurements of the resistance immediately after the formation of the glass as well as slower measurements at low temperatures, where the influence of individual relaxation steps on the resistance can be resolved.

MM 9.27 Mon 18:30 P1

Graphite Composites with Titanium as a Secondary Filler - Microstructure and Electronics — •Hoang Thinh Nguyen, Maria Gaudig, and Ralf Wehrspohn — Martin Luther University Halle-Wittenberg, Institute of Physics, Group μMD, Heinrich-Damerow-Str. 4, 06120 Halle (Saale), Germany

The bipolar plate (BPP) is a crucial component in electrolyzers and fuel cell stacks, serving to separate individual electrochemical cells while ensuring electrical conductivity, water distribution, and mechanical stability. However, the high costs associated with conventional materials like titanium or stainless steel demand the exploration of novel materials and fabrication methods. Graphite-based composites have already emerged as cost-effective alternatives for BPPs. In this work, we developed and characterized an innovative composite material that combines the high electrical conductivity of titanium with the affordability and lamellar structure of graphite to create titanium-graphite composites. Microstructural analyses using scanning electron microscopy (SEM) and nano X-ray computed tomography revealed that titanium particles integrate gapless into the graphite matrix, enhancing the creation of continuous conductive pathways. Electrical conductivity measurements revealed interesting dependencies on filler composition: depending on the filler ratio, either titanium or graphite becomes the dominant contributor to the overall conductivity. These findings highlight the interrelation between particle morphology, structure, and filler ratio in optimizing the composite matrix for BPP applications.

MM 9.28 Mon 18:30 P1

Mesoporous Ti and TiCu network structures prepared by liquid metal dealloying — •Niklas Österle, Markus Ziehmer, Fabian Andorfer, and Carl E. Krill III — Institute of Functional Nanosystems, Ulm University, Germany

Metallic open-cell foams have emerged as promising functional and structural materials. The use of Ti and TiCu would extend the application of such foams into the medical field, as both materials are highly biocompatible, making them excellent choices for implants and prostheses. Combined with the porous structure of metallic foams, which facilitates the infiltration and adhesion of bone cells, the functionality and performance of prosthetic devices could be significantly improved.

In this work, we present the fabrication of mesoporous Ti and TiCu network structures via liquid metal dealloying. This technique enables the selective removal of Cu from TiCu precursor alloys within a Mg melt to form mesoporous structures. By varying the Mg-to-precursor mass ratio, we show that the chemical composition and morphology of the final network can be tailored. The network structure and morphology were investigated using 2D and 3D imaging, and EDS and XRD were employed for phase analysis. Various morphological structures can be linked to specific compounds in the TiCu phase diagram. Future investigations will focus on post-dealloying thermal coarsening.

MM 9.29 Mon 18:30 P1

Role of trace elements on the GP-Zone formation Al-Cu alloys — •Sandra Müller, Isidor Switalla, Johannes Berlin, and Ferdinand Haider — Chair for Experimental Physics I, University of Augsburg, Universitätsstraße 1, 86159 Augsbur

Both formation and dissolution of Guinier-Preston zones in Al-Cu alloys depend on the presence of excess vacancies. They are quenched in from the high temperature homogenisation treatment but will possibly disappear during the natural aging at ambient temperature. The lifetime of excess vacancies in pure Aluminium is much shorter than that in Al-Cu alloys, where vacancies presumably are trapped in GP zones. Therefore, a small increase in temperature can lead to drastic changes in the microstructure of these materials by releasing the trapped vacancies. Resistometry is a simple online method to monitor changes in the microstructure of a metallic alloy, complemented by DSC and hardness measurement.In this work we focused on natural and slightly above room temperature artificial ageing of Al-Cu samples containing 2 - 4 wt.% of Cu. DSC gives rather clear evidence that precursor cluster of only very few atoms form before the GP-zones are detected. Those precursors and the GP zones formation can be suppressed or delayed by minor addition of vacancy-binding trace elements like Tin and Indium.

MM 9.30 Mon 18:30 P1

Irradiation Induced Defects in W-Re Alloys Studied by Positron Annihilation Spectroscopy — •Lisa-Marie Krug[1], Danny Russell[1], Maximilian Suhr[1], Leon Chryssos[1], Lucian Mathes[1], Mikhail Zibrov[2], Thomas Schwarz-Selinger[2], and Christoph Hugenschmidt[1] — [1]Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, 85748 Garching, Germany — [2]Max Planck Institute for Plasma Physics, 85748 Garching, Germany

The plasma-facing components in a fusion reactor have to withstand the irradiation of 14 MeV neutrons, which are released in the fusion reaction of deuterium and trithium. Tungsten is considered to be the most suitable plasma-facing material, due to its high melting point, high thermal conductivity and low erosion under fusion reactor operating conditions. In addition to radiation damage, neutron irradiation of tungsten creates transmutation elements such as rhenium. In this work, the effect of rhenium on the defect characteristics in self-ion irradiated tungsten is investigated. Self-ion irradiation is used to mimic the radiation damage caused by 14 MeV neutrons. Positron annihilation spectroscopy is used to provide non destructive, atomic scale resolution measurement of the irradiation damage. Coincidence Doppler broadening spectroscopy of the 511 keV annihilation line is used to provide element sensitive measurements of vacancy type defects. This allows us to test theoretical predictions that rhenium precipitates around voids.

MM 9.31 Mon 18:30 P1

Phases of AlN by machine learning potentials — •Simon Liebing, Oliver Heymer, and Jens Kortus — Institute of Theoretical Physics, TU Bergakademie Freiberg, Germany

AlN is an important wide-band gap semiconductor with e.g. applications in high power electronics. Under high pressure (about 13 GPa) the wurtzite phase transforms to the rocksalt phase. Here, we attempt to simulate this phase transition as function of temperature and pressure by means of machine learned interatomic potentials trained on accurate density functional theory molecular dynamics data. In particular we will utilize use the open-source library FitSNAP [1] for atomistic machine learning in combination with the molecular dynamics code LAMMPS [2]. FitSNAP is used to provide fast interaction potentials with accuracy inherited from DFT. It already provides interfaces for popular open-source codes such as Quantum ESPRESSO[3], PyTorch and LAMMPS and it supports the state-of-the-art atomic cluster expansion (ACE) descriptors [4]. The ACE descriptors transform structural information into machine learning models. This enables us to carry out large-scale classical MD systems of AlN with thou- sands of atoms with DFT accuracy. The results will be compared to earlier works based on small unit cells using density functional theory. [5] References [1] Rohskopf et al., Journal of Open Source Software, 8 (84), 5118 (2023). [2] A. P. Thompson et al. Comp Phys Comm, 271 10817 (2022). [3] P. Giannozzi et al. J. Chem. Phys. 152, 15 (2020). [4] Drautz, R. Physical Review B, 99 (1), 014104 (2019). [5] S.Schmerler and J. Kortus Physical Review B, 89, 6, (2014).

MM 9.32 Mon 18:30 P1

Brittle to Ductile: Elasticity and Bonding in TiVN Hard Alloys — •Santiago Gómez, Ferenc Tasnadi, Magnus Odén, and Igor A. Abrikosov — Department of Physics, Chemistry and Biology (IFM), Linköping University, Linköping, 58183 Sweden

Hard alloys find extensive applications, such as in coating metal-cutting tools and turbine protective layers, among others. Despite the availability of effective alloys in the market, most remain intrinsically brittle. A critical aspect of alloy engineering is, therefore, the systematic exploration of hard but more ductile alloys with improved fracture toughness.

The low temperature dynamical instability of VN suggest an alloying pathway to improve the ductility of TiN. The idea has been realized by supporting experiments using micro-pillar fracture analysis. In this study, we are searching for novel materials descriptors to gain a better understanding of brittle and ductile behavior, all in an ideal sense suitable for modern data-driven materials science powered by Density Functional Theory (DFT) calculations.

Our findings reveal composition-dependent variations in elastic moduli and anisotropy. Brittle to ductile behavior transition is predicted when a certain composition of Vanadium is reached. Chemical bonding analysis, employing the Quantum Theory of Atoms in Molecules (QTAIM), provide insights into the electronic structure, highlighting trends in bond critical point densities and virial ratios for first-neighbor interactions. These results are contextualized against analogous systems such as $Ti_xAl_{1-x}N$, providing a comparative framework.

MM 9.33 Mon 18:30 P1

Modeling dislocation motion in aluminium alloys by DFT — Inna Plyushchay[1,2], Anna Pliushchai[2,3], Nebahat Bulut[2], Zhengqing Wei[2], and •Sibylle Gemming[2,4] — [1]Natl. Taras Shevchenko University of Kyiv, Ukraine. — [2]Inst. Physics, TU Chemnitz, Germany — [3]Natl. TU of Ukraine, Igor Sikorsky Kyiv Polytechnic Inst., Ukraine — [4]MAIN Center, TU Chemnitz, Germany.

Measured elastic moduli of bulk metals differ from the ideal theoretical values due to the presence of point and line defects as well as grain boundaries, and their joint action has successfully been studied by atomistic simulations. For low-doped alloys with additional elements in small quantities, a plethora of further interactions is obtained, whose classical description is hampered by the lack of suitable potentials for the interaction between different elements. We therefore employ first-principles calculations to determine the dopant-induced electronic structure change in and around the core region of the Shockley partial dislocation in Aluminium as a prototype fcc metal with substitutional Mg, Zr, and Si atoms as dopants. The results indicate that the radius of the first coordination sphere changes within a range of few percent and that all discernible changes in electron density are localized within the first coordination sphere of the impurity. A tendency for the formation of aluminide precipitates is obtained, which may nucleate at 0D, 1D, or 2D defect sites and stabilize local structure motifs which would not be formed in the unperturbed bulk phase.

MM 9.34 Mon 18:30 P1

Generalized susceptibility expressed by Wannier functions — •Dominik Váňa and Jaroslav Hamrle — Faculty of Nuclear Sciences and Physical Engineering, Czech Technical University, Prague

The generalized susceptibility describes the tendency (energy stability) of the cubic phase to become modulated. A typical example is the modulation of Ni_2MnGa [1] which can undergo structural transformation from austenite to a modulated structure. The generalized susceptibility is calculated using occupation probability (Fermi-Dirac distribution), however, this approach omits the dependence which the coupling coefficient of the electron-lattice interaction has on electronic states. The goal of this work is to express generalized susceptibility with calculated coupling coefficients. As the first step, we express generalized susceptibility using Wannier functions, modifying the original approach of Motizuki [2], based on a linear combination of atomic orbitals.

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MM 9.35 Mon 18:30 P1

First-principles insight into the role of electronic band filling on thermodynamic stability and mechanical properties of tantalum-diboride-based solid solutions — •Annop Ektarawong[1], Kunpot Mopoung[1], Chayanon Atthapak[1], Thiti Bovornratanaraks[1], and Björn Alling[2] — [1]Chulalongkorn University, Bangkok, Thailand — [2]Linköping University, Linköping, Sweden

Owing to their superior stabilities and mechanical behaviors at high temperature, AlB_2-type metal diborides have increasingly been considered as promising hard and protective coating materials for cutting tools. In this presentation, we theoretically demonstrate how the thermodynamic stability and mechanical properties of metal diborides can feasibly be improved either through the presence of structural defects beyond the dilute limit or through the alloying process, focusing particularly on tantalum diboride. Our first-principles studies reveal the significant enhancement of the stability, stiffness, shear strength, and hardness of the diboride can directly be interpreted in terms of electronic band filling of the bonding and antibonding states of the material.

MM 9.36 Mon 18:30 P1

Unveiling the Origin of the Yield Stress Anomaly in L12 Intermetallics via Atomistic Approaches — •Xiang Xu, Xi Zhang, and Blazej Grabowski — University of Stuttgart, Stuttgart, Germany

We present an approach to studying the yield stress anomaly (YSA) in L12 intermetallics by bridging the electronic scale with large-scale molecular dynamics simulations, using machine-learning-based interatomic potentials. An ab initio database of temperature-dependent Gibbs energy for relevant planar defects in L12 Ni3Al was developed, covering the full temperature range of the YSA. Machine-learning interatomic potentials for Ni3Al, trained through a physically informed active-learning scheme, achieved accuracy comparable to DFT data and successfully modeled key dislocation behaviors in million-atom models. These MD results enabled the development of a phenomenological model that effectively explains YSA characteristics, offering new insights into the high-temperature performance of L12-strengthened high-entropy alloys.

MM 9.37 Mon 18:30 P1

Modelling and Descriptor-based Synthesizability Analysis of High-Entropy Materials — •Chen-Chen Er[1] and Rico Friedrich[1,2,3] — [1]TU Dresden — [2]Helmholtz-Zentrum Dresden-Rossendorf, Dresden — [3]Duke University, Durham, USA

High-entropy materials (HEMs) are single-phase multi-component disordered systems with unique electronic and thermal properties that are promising for applications in the energy and electronics sectors. HEMs include disordered ceramics such as carbides, nitrides, or oxides with ordered anion sublattices and disorder on the cation sites. There are typically five or more cation species to maximize configurational entropy.

Efficient modelling of the disordered systems is conducted based on an ensemble of supercells approach as implemented in the partial occupation algorithm (POCC) [1] within the AFLOW framework [2,3]. Predictive descriptors including the entropy forming ability (EFA) [4] and disordered enthalpy-entropy descriptor (DEED) [5] are crucial to assess synthesizability. Here, we present results for several high-entropy ceramics, including their electronic properties and synthesizability.

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MM 9.38 Mon 18:30 P1

An extended two-temperature model for copper — •Simon Kümmel and Johannes Roth — FMQ, University of Stuttgart, Germany

Since its introduction, the two-temperature model (TTM) has been a very powerful tool used to simulate material under strong electronic excitation following strong laser irradiation by coupled heat conduction equations for the electronic and lattice system.

Here, we present an implementation of the TTM, coupled to a molecular dynamics code, in which the heat capacity, the heat conduction, electron-phonon coupling parameter depend on the degree of excitation. We extend this model by also including an interatomic potential that depends on the degree of excitation and is capable of reproducing non-thermal effects predicted by electron temperature-dependent density functional theory calculations.

We investigate the influence and importance of each parameter in a case study applied to copper and compare our findings to experimental investigations.

MM 9.39 Mon 18:30 P1

Exploring Ionic Diffusion and Heat Transport Mechanisms in NASICON Materials: A Molecular Dynamics Study — •Insa F. de Vries and Nikos L. Doltsinis — Institute of Solid State Theory, University of Münster, Wilhelm-Klemm-Straße 10, 48149 Münster

In recent years, sodium-ion batteries have emerged as both a potential replacement and a complement to traditional lithium-ion based energy storage systems [1]. However, ensuring the safety and reliability of any future battery system requires a controlled modelling and a thorough understanding of the thermal conduction characteristics, especially with respect to preventing overheating during operation.

Our study uses molecular dynamics calculations on members of the $Na_{1+x}Zr_2Si_xP_{3-x}O_{12}$ family with different stochiometries (x=2.6, 3.4 and 3.8). For each stochiometry we use different cell geometries characterised by an order parameter. In order to reveal the influence of the sodium ion mobility on the heat transport, we calculate key transport properties, namely the sodium diffusion coefficient and the thermal conductivity. We start from a pre-established interatomic potential [2] and calculate the thermal conductivity using a Green-Kubo approach. We find that it peaks for the compounds with $x = 3.4$. Increased diffusion caused by small variations in the parameterisation of the sodium-oxygen interaction leads to simultaneous, equally directed changes in the thermal conductivity.

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MM 9.40 Mon 18:30 P1

Semiclassical transport in multiple Weyl points — •Ricardo Barbosa, Stuart Parkin, and Annika Johansson — Max Planck Institute of Microstructure Physics, Weinberg 2, 06120 Halle (Saale), Germany

We investigate transport contributions[1,2] in three-dimensional materials exhibiting multiple Weyl nodes[2,3], which are linear band touchings acting as point-like sources and sinks of Berry curvature in momentum space, often referred to as "Weyl-Berry monopoles". Specifically, we analyze the transport properties of CoSi[4,5], a chiral topologically nontrivial semimetal with band-touching points of higher-than-twofold degeneracy and nonzero Chern numbers. Notably, at the Γ and R points, the band-touching nodes are four- and six-fold degenerate, respectively, with Chern numbers up to ±4. Using the Boltzmann transport equation[6], we investigate how these features give rise to unconventional electronic properties, focusing on the corresponding charge and node conductivities.

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MM 9.41 Mon 18:30 P1

A novel technique for measuring 3D thermal conductivity of carbon paper — •Oliver Roser[1], Achour Mahfoudi[1], Cornelius Hahn[1], and Andreas Griesinger[1,2] — [1]Center for Heat Management (ZFW), Stuttgart — [2]Baden-Wuerttemberg Cooperative State University (DHBW), Stuttgart

Gas diffusion layers based on carbon paper are used in various types of fuel cells. They make a significant contribution to dissipating the heat loss generated in the catalyst layers and homogenizing the temperature field. The material structure causes strongly direction-dependent thermal conductivities. It is not possible to determine the direction-dependent thermal conductivity under operating boundary conditions using existing methods. We present a newly developed technique with which thermal conductivity can be determined in all spatial directions. Measurements of thermal conductivity in the sample plane are carried out under steady-state boundary conditions. When measuring thermal conductivity through the sample plane, we use a transient measurement approach. The apparatus developed for this purpose and its components are presented. We show how to set and control the application-related boundary conditions such as temperature, surface pressure, moisture content and filling gas. The thermal measurements and evaluation strategies are presented, and the achievable accuracy of the method is discussed. Finally, we show initial measurement results that demonstrate a significant impact of direction, temperature and moisture content on thermal conductivity of gas diffusion layers, depending on the material structure.

MM 9.42 Mon 18:30 P1

Low-temperature thermal conductivity of $YAlO_3$ and $YbAlO_3$ — Parisa Mokhtari[1,2,3], •Ulrike Stockert[3], Stanislav Nikitin[4], Leonid Vasylechko[5], Manuel Brando[2], and Elena Hassinger[3,2] — [1]Department of Physics, Technical University of Munich, 85748 Garching, Germany — [2]Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany — [3]Faculty of Physics, Technische Universität Dresden, 01062 Dresden, Germany — [4]PSI Center for Neutron and Muon Sciences, 5232 Villigen PSI, Switzerland — [5]Lviv Polytechnic National University, Lviv 79013, Ukraine

$YAlO_3$ is a popular substrate, laser, and scintillator material used at temperatures down to those of liquid helium. A good thermal conductivity is required for many applications for instance to facilitate energy release in lasers or thermal coupling via substrates.

We present for the first time thermal conductivity data on $YAlO_3$ below 80 K, covering the T range from 2 K to 300 K. In addition, we have studied the thermal conductivity of YbAlO3 in the temperature window from 50 K to 300 K. Both materials are very good thermal conductors. The thermal transport in these electrical insulators is phononic and can be fitted by the Callaway model. We discuss our results with respect to the relevance of different scattering processes, the origin of the thermal conductivity anisotropy, and the influence of Y-Yb exchange on the thermal transport. Our results on $YAlO_3$ confirm the suitability of the material for applications requiring a low thermal resistance at temperatures down to liquid He.

MM 9.43 Mon 18:30 P1

(Very) high-temperature physics of selected Planckian metals — •Zuzanna Helena Filipiak[1,2] and Andrew P. Mackenzie[1,2] — [1]Max-Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]Scottish Universities Physics Alliance, School of Physics and Astronomy, University of St Andrews, United Kingdom

Planckian dissipation is the mysterious phenomenon of an almost universal saturation of the electron scattering rate in many condensed matter systems despite their vastly different microscopics and strengths of electron interactions. In crystalline samples, the Planckian temperature dependence of resistivity is referred to as strange metallicity in the low-temperature regime and bad metallicity if the behaviour continues to high temperatures. Despite interest in such materials because of their unique physics, their high-temperature characteristics continues to be understudied. We developed two setups in which resistivity of a metallic sample is measured as a function of temperature (ranging from 2 to 1000 K), magnetic field (up to 12 T) and atmosphere (oxygen-rich, argon, high vacuum). Our results for selected single-crystal and thin-film samples of metallic delafossites, nickelates and ruthenates, incl. ruthenium dioxide, will be presented.

MM 9.44 Mon 18:30 P1

Fitting Tensorial Properties with MACE: a Study of $Li_2Ti_5O_{12}$ Electric Field Gradient Tensors — Elena Gelzinyte[1], Karsten Reuter[1], Christian Carbogno[1], and •Johannes T. Margraf[2] — [1]Fritz-Haber-Institut der MPG, Berlin — [2]University of Bayreuth

Machine learning interatomic potentials, which serve as surrogate models for predicting a structure's energy and forces, have significantly accelerated atomistic simulations. Equivalent approaches have been applied to predict other structural or atomic properties, such as charges, dipole moments, and polarisabilities. One such framework is MACE, a higher-order equivariant neural network [1]. Due to the way its internal features are constructed, the output part of the model may be readily modified to suit the symmetry of the target property. In this presentation, we discuss the required modifications for fitting atomic tensorial quantities and the resulting model's applicability, limitations, and advantages. For illustration, we focus on the prediction of electric field gradient tensors (a per-atom traceless symmetric tensor) using a $Li_2Ti_5O_{12}$ data set [2]. We consider the improvement in fitting the tensorial properties directly, rather than derived scalar properties, and compare the modified MACE's results with those of λ-SOAP [3], discussed in [2].

[1] I. Batatia *et al.*, NeurIPS **35**, 11423 (2022).

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[3] A. Grisafi *et al.*, Phys. Rev. Lett. **120**, 036002 (2018).

MM 9.45 Mon 18:30 P1

First-Principles Analysis of Spin-Disorder Resistivity and Its

Temperature Dependence — •Fabian Engelke, Felix Schug, Michael Czerner, and Christian Heiliger — Justus-Liebig-Universität, Giessen, Germany

By means of Matthiessen's rule, one can decompose the electrical resistivity of materials into contributions of separate scattering mechanisms. Here, we present ab initio calculations of the electron-magnon scattering contribution to the specific resistivity of ferromagnetic materials within the supercell method. For that purpose, we model the spin disorder with an atomistic spin model described by a Heisenberg Hamiltonian. We then use the Landau-Lifschitz-Gilbert equation to describe the system's dynamics and introduce temperature effects utilizing Langevin dynamics. In the second step, we employ noncollinear density functional theory and the Non-equilibrium-Green's function formalism in a Koringa Kohn Rostocker (KKR) representation to calculate the conductance through slabs of varying thickness derived from the spin-configurations obtained in the first step. Subsequently, we calculate the specific resistivity by averaging over supercells and applying Ohm's Law. First results for Fe show good agreement with experimental data at high temperatures, highlighting the contribution of magnetic short-range order effects to the total temperature dependence of the specific electric resistance in the temperature regime above the Curie-Temperature.

MM 9.46 Mon 18:30 P1

Tuning intrinsic anomalous Hall effect from large to zero in two ferromagnetic states of SmMn$_2$Ge$_2$ — Mahima Singh[1], Jyotirmoy Sau[1], •Banik Rai[1,2], Arunanshu Panda[1], Manoranjan Kumar[1], and Nitesh Kumar[1] — [1]S N Bose National Centre for Basic Sciences, Salt Lake City, Kolkata 700106, India — [2]Leibniz Institute for Solid State and Materials Research (IFW) Dresden, Helmholtzstraße 20, 01069 Dresden

The intrinsic anomalous Hall conductivity (AHC) in a ferromagnetic metal is determined by its band structure, with spin orientation being a key band structure tuning parameter. We study a layered tetragonal room temperature metallic ferromagnet SmMn$_2$Ge$_2$, which gives us the opportunity to study magneto-transport properties where both the c-axis and a-axis can be magnetically easy axes depending on the temperature range we choose. We show a moderately large fully intrinsic AHC up to room temperature when the crystal is magnetized along the c-axis. Interestingly, the AHC can be tuned to completely extrinsic with extremely large values when the crystal is magnetized along the a-axis, regardless of whether the a-axis is magnetically easy or hard. First principles calculations show that nodal line states originate from Mn-d orbitals just below the Fermi energy (E_F) in the electronic band structure when the spins are oriented along the c-axis. Intrinsic AHC originates from the Berry curvature effect of the gapped nodal lines in the presence of spin-orbit coupling. AHC almost disappears when the spins are aligned along the a-axis as the nodal line states shift above E_F and become unoccupied.

MM 9.47 Mon 18:30 P1

Rapid photobleaching of Yb-doped optical fibers exposed to gamma radiation by high energy ns pulsed laser — •Esra Kendir Tekgül and Bülend Ortaç — Bilkent University UNAM, Institute of Materials Science and Nanotechnology, Ankara, 06800, TURKEY

Rare earth-doped optical fibers (OFs) have become one of the new high-power laser and sensor applications. Therefore, it is very important to protect such OFs from being exposed to external effects and to increase their reusability after these effects. Here, Radiation Induced Attenuation (RIA) and the Photo-darkening (PD) processes play an important role. The main source of the problem is the color centers formed in the OF. Preventing or recovering these formations before and after the production of OF is of great importance in both efficient and long-lasting systems.

To determine the behavior of Yb-doped OF, they are exposed to gamma radiation or PD. The important recovery process is photobleaching (PB) for defects due to the gamma radiation. In our study, a rapid and efficient PB process was achieved using a high-energy nanosecond pulse to recover existing and/or revealed color centers in OF that had been irradiated with 10 kGy of gamma radiation. The PB process was analyzed based on the wavelength and energy of the pulsed light source. The highest level was achieved with the 532 nm wavelength laser. The findings indicate that the recovery of color centers can reach up to 96% in a shorter duration (hours) compared to results from studies utilizing continuous lasers.

MM 9.48 Mon 18:30 P1

Design of a setup for conducting experiments synchronized with sample scanning — •Maksim Khasanov — Moscow, Russia

The paper focuses on designing equipment with an electronic drive for compressing samples during experiments, aimed at analyzing their internal structure using computed tomography. The manual compression system previously used prolonged the experiment due to time-consuming data processing. The new electronic system significantly reduces the time required by automating the compression process. The work includes the design of the compression apparatus and its electric drive, providing a more efficient and precise solution for experimental procedures.

MM 9.49 Mon 18:30 P1

Extreme stability of CoCrFeMnNi$_{60}$ multicomponent alloys after severe plastic deformation — •Lukas Musiol[1], Mohan Muralikrishna Garlapati[1], Shabnam Taheriniya[1], Lukasz Rogal[2], Sergiy Divinskiy[1], Harald Rösner[1], and Gerhard Wilde[1] — [1]Institute of Materials Physics, University of Münster, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany — [2]Institute of Metallurgy and Material Science, Polish Academy of Science, Reymonta 25 St., 30-059 Krakow, Poland

Thermal stability of a (CoCrFeMn)Ni60 multicomponent alloy is investigated using in-depth microscopic examination. The specific composition is chosen as a transition one from “high-entropy” to “concentrated alloy” behavior. Such compositional design mimics a conventional alloy design of solutes in the terminal solid solution range but in equiatomic concentrations. Along with the analyses of the homogenized samples, an analysis of compressed and rotary swaged samples was performed to investigate the influence of deformation on the phase stability. The phase stability is investigated at intermediate temperature for prolonged annealing times, which has given an in-depth understanding of the formation and growth of new phases or precipitates. Detailed microscopy analyses were performed to determine the phases and their composition. Overall, the (CoCrFeMn)Ni60 multicomponent alloy has shown a stable microstructure even after extreme deformation and after prolonged heat treatments. The phase stability results, in conjunction with deformation and microstructure, will be correlated and discussed in detail.

MM 9.50 Mon 18:30 P1

Influence of Supercell Size Effects on the Mechanical Properties and Electronic Structure of High-Entropy Transition Metal Diborides (HETMB$_2$) — Inna Plyushchay[2], •Nebahat Bulut[1], Anna Pliushchai[1,3], and Sibylle Gemming[1] — [1]Institute of Physics, TU Chemnitz, Germany — [2]Institute of Physics, National Taras Shevchenko University of Kyiv, Ukraine — [3]National Technical University of Ukraine "Igor Sikorsky Kyiv Polytechnic Institute"

Modeling various supercell sizes for high-entropy transition metal diborides (HETMB$_2$) holds the potential to overcome the computational challenges associated with their unique bonding configurations and complex compositions. First-principles calculations were used to predict the electronic and elastic properties of high-entropy transition-metal diborides after employing supercells with a variety of atomic configurations and complex compositions. We found that larger supercells allowed for clustering of atoms of the same metal type, as evidenced by broadening of the peaks in the histogram of interatomic distances. This, however, had no significant influence on the mechanical properties. The mechanical properties of HETMB$_2$ are determined by the number of electrons, size of atoms or polarizability. However, the average number of d-electrons per metal atom was found to be crucial because it affects the Fermi level position relative to the pseudogap, and this impacts the elastic properties strongly in comparison to the binary-TMB$_2$.

MM 9.51 Mon 18:30 P1

Ab initio calculations of defects in the Mg2Ge intermetallic — •Pavel Papež[1,2], Martin Friák[2], and Martin Zelený[1] — [1]Institute of Materials Science and Engineering, Faculty of Mechanical Engineering, Brno University of Technology, Brno, Czech Republic — [2]Institute of Physics of Materials, Czech Academy of Sciences, v. v. i., Brno, Czech Republic

This work is focused on ab initio calculations of different types of defects in the Mg2Ge intermetallic in order to explain a higher concentration of Mg in experimental samples. Our calculations employed VASP software and include antisite defects and vacancies on both sublattices and furthermore interstitial additions of both Mg and Ge, all in charge neutral state. The calculations were also done with the modified Becke-Johnson potentials to study their influence on the bandstructure of this semiconductor. We have calculated their formation energies in regards to Mg rich and Ge rich chemical potential limits. The phonon calculations were done to acquire the defect equillibrium concentration and the evolutiuon of defect formation energies with temperature.

MM 9.52 Mon 18:30 P1

Glass transition and physical aging studies of a gold based Bulk metallic glass by means of flash scanning calorimetry — •Klara Otto[1], Valerio Di Lisio[2], Daniele Cangialosi[2], and Isabella Gallino[1] — [1]Technische University Berlin, Chair for Metallic Materials, Berlin, Germany — [2]DIPC, San Sebastián, Spain

Flash scanning calorimetry is used to study the glass transition of metallic glasses, during direct solidification from the melt [1,2] and by reheating with rates up to thousands of K/s. This enables the access to the supercooled liquid state by avoiding crystallization during the cooling stages.

Glassy materials relax over time when held below the glass transition temperature, to minimize their excess thermodynamic properties. A new methodology to compare the relaxation times related to the atomic mobility with those determined throughout glassy aging of a gold based metallic glass, is presented. Isothermal physical aging was performed to retrieve the temperature dependent timescales of the alpha relaxation. Additionally, the characteristic time of glassy relaxation are retrieved in a wide temperature range [3] complemented with fictive temperature analysis.

The combined data were plotted on an activation diagram, that relates relaxation times to the inverse of temperature. This allowed to investigate relaxation time scales spanning 7 orders of magnitude using a single experimental technique.

[1] Di Lisio, V,(2023),Nat. Commun.,14(1),[2] Monnier, X,(2020),Sci. Adv.,6(17),[3] Gallino, I,(2018), Acta Mater.,144

MM 9.53 Mon 18:30 P1

Glass Forming Ability, Thermal and Magnetic Properties of the Multicomponent Fe-Mo-P-C-B-Si Metallic Glass for AM Applications — •Alejandro Lejtman Rotberg[1], Amirhossein Ghamivi[2], Lucas M. Ruschel[2], Izzi A. Ahmad[1], Uma Rajput[3], Purbasha Sharangi[3], Paola M. Tiberto[2], Ralf Busch[2], and Isabella Gallino[1] — [1]Technical University of Berlin, Chair for Metallic Materials, Ernst-Reuter-Platz 1, 10587 Berlin, Germany — [2]Saarland University, Chair of Metallic Materials, 66123 Saarbrücken, Germany — [3]INRIM, Strade delle Cacce 91, Torino, Italy

Efficient power-to-work conversion in electric vehicles (EVs) requires soft magnetic materials with low coercivity. Fe-based metallic glasses reduce power losses but struggle achieving casting thicknesses over 1mm due to limited glass-forming ability (GFA). Additive manufacturing (AM), like Laser Powder Bed Fusion (LPBF), provides solutions, with recent studies revisiting Fe-Si-B compositions for processability and performance [1-3]. This study evaluates the alloy Fe74Mo4P10C7.5B2.5Si2. X-ray diffraction (XRD) results of cast plates and ribbons determined the GFA. Thermal properties were analyzed via Differential Scanning Calorimetry (DSC) and Differential Thermal Analysis (DTA), while magnetic properties using Vibrating Sample Magnetometry (VSM). Results suggest the alloy's potential for AM production of soft magnetic components for EVs.[1] Thorsson, L., et al. Selective Laser Melting. Materials & Design.[2] Rodríguez-Sánchez, M., et al. Relating Laser Powder. Materialia.[3] Sadanand, S., et al. Laser Powder Bed Fusion. Journal of Laser Applications.

MM 9.54 Mon 18:30 P1

An atomistic study on the role of size and composition on the structural and thermodynamic properties of Al-Pd bimetallic nanoparticles during melting and solidification. — •Dario Gonzalo Escriba Quispe[1], Justo Alcides Rojas Tapia[1], and Gustavo Cuba Supanta[1,2] — [1]Universidad Nacional Mayor de San Marcos, Lima, Peru — [2]Universidad Privada del Norte, Lima, Peru

Bimetallic nanoparticles (NPs) of Al-Pd exhibit structurally complex phases, as well as quasicrystalline approximants to the Al-Mn-Pd system, which, combined with their controversial and complex phase diagram, makes them an interesting subject of study. In this work, using molecular dynamics, the structural and thermodynamic properties of Al(x)Pd(100-x) NPs at different sizes and compositions are calculated.

The processes of melting and solidification are simulated using the open-source LAMMPS package and a MEAM-type potential. It was found, through the calculation of heat capacity, that the melting temperature and size of AlPd, Al2Pd5, and Al1Pd4 NPs follow a linear behavior, in agreement with the scaling law. Additionally, the RDF graphs of AlPd NPs show that it is an ordered intermetallic compound, with structural parameters such as the crystal structure and lattice parameter matching those reported experimentally. The Al1Pd4 nanoalloy was explored, where it was found that the NP has an icosahedral shape. However, the atoms exhibit internal ordering with regions showing FCC and HCP crystal structures. Finally, other additional results such as MSD, common neighbor analysis (CNA), the Warren-Cowley parameter, excess energy, and phonon dispersion are presented.

MM 9.55 Mon 18:30 P1

An X-ray diffraction study of copper powder for laser-based powder bed fusion — •Eric Schneider[1], Robert Ortmann[2], Julia Frank[3], Fabienne Hellwig[3], Tobias Grimm[2], Michael Blüm[3], Lena Friedrich[1], Michael Paulus[1], Jaqueline Savelkouls[1], Jan T. Sehrt[2], Christian Sternemann[1], and Arne Röttger[3] — [1]Universität TU Dortmund, Maria-Goeppert-Mayer-Straße 2, D-44227 Dortmund — [2]Ruhr-Universität Bochum, Universitätsstraße 150, D-44801 Bochum — [3]Bergische Universität Wuppertal, Bahnhofstraße 15, D-42651 Solingen

Additive manufacturing (AM) of components using laser-based powder bed fusion of metals (PBF-LB/M) has reached market maturity. This layer-by-layer process offers advantages over casting and subtractive methods, especially for producing complex parts with internal cavities and is promising to produce topology-optimized lightweight structures. However, the use of copper powders for PBF-LB/M based AM poses challenges due to its high thermal conductivity and reflectivity. The directed oxidation and reduction of the copper particle surfaces can improve both, the powders processability and reusability. In this study we investigate the oxidation of pre-treated copper powders in air and its controlled reduction using $\mathrm{Ar/2\%H_2}$ atmosphere at different temperature conditions up to 350°C by X-ray diffraction at beamline BL9 of DELTA synchrotron radiation source in order to reveal information about induction times and change in Cu, $\mathrm{Cu_2O}$, and CuO phase composition for industrial processing. This research is funded by the DFG via projects RO 4523/9-1, SE 2935/6-1, and STE 1079/9-1.

MM 9.56 Mon 18:30 P1

Linking Process Parameters and Heat Treatment to Microstructural Properties of PBF-LBM 316L Steel for Structural Hydrogen Use — •Tim Haag, •Kai Stefan Lagemann, Stefan Wagner, and Astrid Pundt — Institut für Angewandte Materialien - Werkstoffkunde (IAM-WK), Karlsruher Institut für Technologie (KIT)

Additively manufactured (AM) 316L steel produced by powder bed-based laser melting (PBF-LBM) can be considered for sophisticated applications in hydrogen technology. This project investigates the influence of manufacturing parameters and post-processing treatments, such as heat treatment, on the resulting microstructure and its implications for material properties. The objective is to optimise the manufacturing process in order to achieve components with minimal porosity. The microstructure is comprehensively analysed using advanced techniques, which reveal hierarchical features and a complex interplay of various microstructural elements, including multiscale porosity, varying grain orientations and subgrain dislocation cells. Heat treatments are applied to alter microstructural characteristics and assess their impact on material properties.

MM 9.57 Mon 18:30 P1

Analysis of the Crack Formation in Printed Nanosilver Using In Situ Bending Technique — •Lennart Schwan[1], Michaela Klöcker[1], Michael Feige[1], Laila Bondzio[2], Thomas Kordisch[1], and Sonja Schöning[1] — [1]Bielefeld Institute for Applied Materials Research (BIfAM), Faculty of Engineering and Mathematics, Bielefeld University of Applied Sciences and Arts — [2]Thin Films & Physics of Nanostructures, Bielefeld University, Department of Physics

3D printing is an emerging technology with a wide range of applications. The modern multi-material jetting process, as used in the Nano Dimension Dragonfly Pro LDM, makes it possible to print dielectric and conductive materials in a single process. In addition to electrical circuits such as coils, capacitors, etc., strain gauges can also be printed.

The change in resistance of strain gauges is usually caused by the change in the geometric dimensions of the conductive layer when it is deformed. In the case of the printed material examined in this study, it is also known that the material is permeated by cracks which cause a directional dependence of the electrical conductivity.

The objective of this study is to investigate how these cracks develop during bending and thus also contribute to the change in resistance. For this purpose, a test specimen is loaded under a three-point bending test using a special in situ bending module. In order to investigate the propagation and formation of the cracks, the bending module is positioned in a scanning electron microscope in order to analyze the cracks under loading with a sufficient image resolution.

MM 9.58 Mon 18:30 P1

Atomistic Simulation of Laser-based Powder Bed Fusion of Metals — •Aamir Siddiqui, Simon Kümmel, and Johannes Roth — FMQ, University of Stuttgart, Germany

Additive manufacturing technology applications continue to call for increased reproducibility and quality. The goal is to study the melting and solidification of an AlTi alloy and to create a framework that allows for further studies on arbitrary alloys and metals. Molecular dynamics provides an understanding of the melting and ablation process, resulting in an understanding of different heat transfer mechanisms. The simulation framework makes it possible to see how changes in scanning speed and laser power affect the melting dynamics.

The melting process of alloys shows that a significant amount of argon gas becomes trapped inside the sample. The simulation of powder beds formed by spheres of varying sizes reveals holes that vanish under vacuum conditions, but persist when the simulation box is filled with protective gas, providing information on the creation of defects. By deforming the sample, the influence of gas pockets on the mechanical properties and the evolution of the lattice structure within the sample can be seen.

MM 9.59 Mon 18:30 P1

Nanoscale characterization of AM316L stainless steel for hydrogen application — •Gabriele Palazzo, •Felix Stierle, Kai Stefan Lagemann, Christian Kübel, Stefan Wagner, and Astrid Pundt — Karlsruhe Institute of Technology, Karlsruhe, Germany

Additive manufactured (AM) austenitic stainless steel 316L prepared by selective laser melting (SLM) is characterized by advanced nanoscale characterization techniques to examine its microstructural features. High-resolution scanning TEM (HR-STEM), selected area diffraction (SAD), and analytical methods such as energy-dispersive X-ray spectroscopy (EDX) as well as electron energy loss spectroscopy (EELS) are employed. Typical SLM printing structures (equiaxial and columnar cellular structure, nano-inclusions) are observed with atomic resolution both for as-built and tensile tested samples. The presence of silicon-manganese oxide nano-inclusions, preferential chromium and molybdenum segregation around them is revealed, as well as iron depletion and chromium enrichment along the cell boundaries. This peculiar multi-scale AM microstructure accounts for the unique mechanical properties of AM316L in terms of resistance and ductile behaviour, if compared to the conventionally manufactured counterpart, allowing to overcome the trade-off between strength and ductility.

MM 9.60 Mon 18:30 P1

Fine-tuning of machine learning interatomic potential for the prediction of phonon properties — •Jonas Grandel, Philipp Benner, and Janine George — Bundesanstalt für Materialforschung und Prüfung, Berlin

Accurate phonon predictions are critical for assessing material stability and thermal behavior, but traditional approaches based on density functional theory (DFT) are computationally expensive, motivating the need for accelerated alternatives. In this work, we investigate the performance of the machine learning interatomic potential MACE-MP-0 for predicting harmonic phonons and thermal properties. The focus is on fine-tuning MACE-MP-0 using various sets of rattled structures and different hyperparameter to identify the most effective strategy for improving model accuracy. We want to develop a general fine-tuning workflow based on the foundational model that can be used to fast and accurately generate phonons to predict both stability and thermal properties. For this purpose, a benchmark dataset was constructed using DFT consisting of a broad range of different crystal systems and mainly of phase change materials and thermoelectric materials. Each fine-tuned model targets one specific material, allowing to improve each material individually. The results demonstrate significant improvements in the prediction of phonon band structures, with a root mean square error (RMSE) reduced from 0.6 THz for the original MACE-MP-0 model to 0.3 THz for the fine-tuned models. In addition, performance in terms of computational speed was improved by up to a factor of 10 compared to traditional DFT-based phonon calculations.

MM 9.61 Mon 18:30 P1

Learning the Reduced Density Matrix Functional from Quantum Processors and Using Density Matrix Embedding Theory to Extend its Universality — •Martin Uttendorfer — Deutsches Zentrum für Luft- und Raumfahrt (DLR), Köln, Deutschland

The advent of quantum computing makes reduced density matrix functional theory (RDMFT) on an exact level viable. By directly applying RDMFT, derived from Levy-Lieb's constrained search, this work leverages quantum processors to overcome some of DFT*s shortcomings, enabling more accurate modeling of quantum chemical and condensed matter systems. The proposed approach incorporates quantum algorithms that utilize variational quantum eigensolvers (VQE), which is viable to be executed on near-term intermediate scale quantum devices (NISQ) in conjunction with machine learning techniques. This work examines the theory*s application to different particle types, including fermions, bosons, and hard-core bosons, highlighting the flexibility of the RDMFT framework. Additionally, density matrix embedding theory (DMET) is incorporated, allowing for a hybrid classical-quantum approach that extends the functional*s universality. This work presents a quantum algorithmic approach to obtain the functional and provides a computational strategy for studying complex many-body systems while keeping the use of limited quantum resources to a minimum.

MM 9.62 Mon 18:30 P1

Integrating Long-Range Interactions into Machine Learning Interatomic Potentials — •Tulga-Erdene Sodjargal[1,2], Egor Rumiantsev[1], Philip Loche[1], and Michele Ceriotti[1] — [1]Laboratory of Computational Science and Modeling (COSMO), Institute of Materials, École Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland — [2]Department of Bio and Brain Engineering, Korea Advanced Institute of Science and Technology (KAIST), 34141 Daejeon, Republic of Korea

Machine learning-based interatomic potentials (MLIPs) often rely on the locality ansatz, calculating atomic energies based on a fixed cutoff radius. While effective for many systems, this nearsightedness can lead to inaccuracies when long-range interactions, such as ionic interactions, dominate. To overcome this limitation, we integrate Particle Mesh Ewald (PME) techniques into existing MLIP frameworks. Our extension is modular and plug-and-play, requiring minimal modifications to incorporate into various models. We demonstrate significant improvements in both simple architectures, such as Behler-Parrinello Neural Networks, and advanced models, including state-of-the-art graph neural networks like the Point Edge Transformer (PET).

MM 9.63 Mon 18:30 P1

pyiron - Automated Workflows for Materials Science — •Jan Janssen[1], Marvin Poul[1], Sarath Menon[1], Tilmann Hickel[2], and Joerg Neugebauer[1] — [1]MPI for Sustainable Materials, Düsseldorf, Germany — [2]BAM Federal Institute for Materials Research and Testing, Berlin, Germany

The pyiron framework, originally developed for atomistic simulations in the field of materials science, has recently been extended beyond the atomistic scale to enable data-driven materials design on all scales and including experiments. As a central interface for materials acceleration platforms (MAP), pyiron couples simulation methods ranging from ab-initio methods of the electronic scale, to the atomistic scale of machine-learned interatomic potentials and up to the continuum scale of crystal plasticity modelling with interfaces for experimental equipment and machine learning.

On our poster, we give a brief overview of the recent developments in the pyiron project and highlight a series of materials science applications. These range from pyiron_workflow, our redesigned graph-based workflow engine, to executorlib for up-scaling workflows for high-performance computing (HPC) and the python workflow definition, a joined standard developed in collaboration with AiiDA and jobflow, the workflow engine of the materials project. At the same time, the poster will provide an opportunity to meet the pyiron developers and discuss ideas and future applications.

Read more about pyiron on our website: https://pyiron.org

MM 9.64 Mon 18:30 P1

Investigating the Impact of Optimization Algorithms on

Element-Substitution Based Materials Discovery — •David Greten[1], Konstantin Jakob[1], Karsten Reuter[1], and Johannes T. Margraf[2] — [1]Fritz-Haber-Institut der MPG, Berlin — [2]University of Bayreuth

In this study, we investigate how different optimization algorithms affect the relaxation of inorganic structures using general-purpose machine-learned interatomic potentials (MLIPs) like MACE-MP-0. Assessing computational efficiency and relaxation quality via structural similarity and kernel distance metrics, we find that optimizer choice significantly influences performance and can lead to different equilibrium structures. Analyzing both DFT-relaxed structures from the Materials Project and element-substitution based trial structures, we highlight the optimizer's impact in different scenarios. Our findings emphasize the critical role of optimizer selection in large-scale computational materials science workflows, particularly in the context of element-substitution based materials discovery. This can hopefully guide the community towards choosing appropriate algorithms for efficient and reliable structure relaxations.

MM 9.65 Mon 18:30 P1

The APyT Package: From Raw Data to Three-Dimensional Reconstruction — •Sebastian Eich — Department for Materials Physics, Institute for Materials Science, University of Stuttgart

The APyT package is an advanced, open-source Python framework for evaluating atom probe tomography (APT) data. It offers a suite of modules that automate key steps in APT processing, from mass spectrum calibration to three-dimensional sample reconstruction. Its modular architecture ensures seamless integration with external tools through standardized input/output interfaces, supporting both Linux and Windows environments.

Key features include high efficiency with NumPy and Numba, a low memory footprint, and extensive documentation. The modules are highly automated, requiring minimal user input to achieve accurate results. The package also integrates SQL database management for raw measurement data and corresponding metadata.

The mass spectrum module automatically calibrates and detects peaks, producing high-resolution spectra. The mass spectrum fitting module further refines this by fitting spectra with an analytical function, automatically de-convolving overlapping peaks by incorporating isotope abundances. The reconstruction module generates a 3D sample reconstruction, including automatic chemical identification and export capabilities. Future enhancements include a PyQt-based GUI to streamline access to all APyT modules in one application.

MM 9.66 Mon 18:30 P1

Relation between the electronic structure and X-ray absorption spectra discussed using multiple-scattering formalism — Hubert Ebert[1], •Sergiy Mankovsky[1], and Jan Minar[2] — [1]LMU of Munich, 81377 Munich, Germany — [2]University of West Bohemia, Pilzen, Czech Republic

Recently, the concept of crystal orbital overlap population (COOP) has been reconsidered [1] based on the finite difference method (FDM), representing the calculated x-ray absorption spectra (XAS) in terms crystal orbital overlap population functions. This allows to reveal the correlation between XAS and the formation of the bonding/antibonding states in solids. Following the idea suggested in Ref. [1], we demonstrate that this relation can be investigated in a very efficient way using the multiple scattering formalism for electronic structure calculations. In this representation, both, the density of states and the x-ray absorption function are determined by the site-diagonal scattering path operator $\tau^{00}(E)$ which can be expressed as $\tau^{00}(E) = t^0 + \sum_n \tau^{0n}(E)\, G^{n0}(E)\, t^0$, in terms of the single-site scattering matrix t^0, the site-off-diagonal operators $\tau^{0n}(E)$, and the structural Green function $G^{n0}(E)$. The second term determines in a pair-wise resolved way the fine structure of the electron density of states (DOS) $n(E)$ as well as the XAS absorption coefficient $\mu(E)$. The DOS and the normalized x-ray absorption coefficient are calculated for several representative systems and discussed in line with the idea of the COOP concept.

[1] M. Diaz-Lopez, *et al.*, J. Phys. Chem. A **124**, 6111 (2020)

MM 9.67 Mon 18:30 P1

Upgrading the Coincidence Doppler Broadening Spectrometer at FRM II — •Danny R Russell, Francesco Guatieri, Leon Chryssos, and Christoph Hugenschmidt — FRM II - Technische Universität München, München, DE

The coincidence Doppler broadening spectrometer (CDBS) at the Forschungs-Neutronenquelle Heinz Maier-Leibnitz (FRM II) provides state-of-the-art, depth dependent detection of defects and chemical composition at the annihilation site. A monoenergetic positron microbeam (50 μm FWHM) is guided onto a sample where positrons annihilate with electrons. The Doppler broadening of the characteristic 511 keV annihilation peak is measured by observing both emitted photons simultaneously.

We present simulations and hardware design for an upgrade to the CDBS which will allow backscattered positron capture. Up to ~ 40 % of the incident positrons are backscattered when they reach the sample surface. The annihilation events occurring when these backscattered positrons return to the sample or annihilate in experimental hardware contribute unwanted signal to the measured spectrum which cannot be removed in data processing.

We use an in-house particle tracking code to design a positron dump that will capture backscattered positrons at an electrode outside detector lines of sight. This will reduce the unwanted signal by up to 50 % and improve the quality of CDBS data. Additionally, we apply the same code to optimize an electrostatic focusing lens, further increasing the spatial resolution of the instrument.

MM 9.68 Mon 18:30 P1

High-entropy alloy pre-screening for lead-free halide double perovskites from material databases — •Marina S. Günthert[1,2], Bernd Meyer[1], and Christoph J. Brabec[2] — [1]Interdisciplinary Center for Molecular Materials and Computer Chemistry Center, FAU Erlangen-Nürnberg — [2]Materials for Electronics and Energy Technology (i-MEET), FAU Erlangen-Nürnberg

Over the last decade, lead-free halide double perovskites with composition $A_2BB'X_6$ have emerged as an interesting class of materials for optoelectronics. Furthermore, it was suggested to introduce different ion ratios on each of the double perovskite sublattices, leading to a vast space of possible compositions.

Two criteria are applied to have a first fast filtering approach to reduce the number of combinations. First, the search is limited to non-toxic and non-f elements for a green chemistry approach. Second, we estimate the thermodynamic stability of the compounds by using a criteria recently proposed by Muzzillo *et al.* [1], which focuses on the entropy stabilization by using several elements on each sublattice. This method can be easily adjusted for halide double perovskites. We applied it first to the Materials Project database but it can also be extended to other databases such as NOMAD and OQMD. In the end, this pre-screening gives an idea, which elements on the different sublattices of the double perovskite are worth further exploration.

[1] C.P. Muzzillo, C.V. Ciobanu, D.T. Moore, High-entropy alloy screening for halide perovskites, Mater. Horiz. **11** (2024) 3662-3694

MM 9.69 Mon 18:30 P1

Effect of $4f$ occupancy on L_3 edge of Cerium — •Prathibha Chandrashekhar, Patrik Thunström, Felix Sorgenfrei, and Heike Herper — Department of Physics and Astronomy, Uppsala University, Sweden

The valence $4f$ electrons in Cerium exhibit a strong itinerant tendency, allowing them to exist in a mixed-valence regime, between localized and delocalized states. This regime hosts correlated electron phenomena which has profound implications on the material's magnetic, transport, and electronic properties. The shift in $5d$ orbitals to higher energy levels, due to reduced screening from delocalized $4f$ electrons, provides critical insights into electronic properties. We study this shift by probing $2p$ to $5d$ transition using X-ray Absorption Spectra(XAS). However, accurately modeling the light-matter interaction in such systems remains challenging due to the itinerant nature of the $4f$ electrons, strong core-hole effects, multiplet interactions, and hybridization dynamics. In this work, we employ advanced theoretical approach that combines density functional theory (DFT) with multiplet ligand-field theory (MLFT). This method enables computation of $L_{2,3}$-edges by constructing and solving single-impurity Anderson model (SIAM) derived from first-principles calculations. Additionally, we investigate sensitivity of the computed spectra to Slater integrals, hybridization effects, and core-hole relaxation, offering new insights into the intricate electronic behavior of Cerium-based systems. PC acknowledges partial funding from Horizon Europe MSCA Doctoral Network grant n.101073486, EUSpecLab, funded by European Union.

MM 9.70 Mon 18:30 P1

Stability of AgI Polymorphs and the AgI(0001) Surface

Reconstruction — •Angela Rittsteuer[1], Andrea Conti[2], Michael Schmid[2], and Georg Kresse[1] — [1]University of Vienna, Faculty of Physics, 1090 Vienna, Austria — [2]TU Wien, Institute of Applied Physics, 1040 Vienna, Austria

Silver iodide (AgI) is a compound widely used in cloud seeding due to its ability to act as an effective nucleating agent for cloud condensation. Under ambient conditions, AgI crystallizes in hexagonal or cubic close-packed structures, the most prominent polymorphs being the wurtzite and the zincblende structure. A comprehensive understanding of its groundstate structures and phase behavior is essential not only to optimize its role in cloud condensation but also to explore broader applications in solid-state chemistry and catalysis.

To investigate the stability of AgI polymorphs, we perform extensive benchmarking studies across various levels of theory. These include Density Functional Theory with different approximations for the exchange-correlation energy, hybrid Hartree-Fock Density Functionals, and the Random Phase Approximation, offering a hierarchy of accuracy. Building on recent atomic force microscopy studies of the wurtzite AgI(0001) surface, we further provide theoretical insights by developing a machine-learned force field and applying simulated annealing and parallel tempering to study the surface reconstruction.

MM 9.71 Mon 18:30 P1

Investigation of Lloyd's formula at finite electronic temperatures — •Christian Maas[1,2], Michael Czerner[1,2], and Christian Heiliger[1,2] — [1]Institut für Theoretische Physik, Justus-Liebig-Universität Gießen — [2]Center for Materials Research (LaMa), Justus-Liebig-Universität Gießen

In DFT calculations within the Korringa-Kohn-Rostoker (KKR) Green's function formalism the integrated density of states is analytically given by Lloyd's formula. Its better l-convergence can be used for a precise determination of the Fermi energy and a charge density normalization. In the past it has been shown that for finite electronic temperatures the calculation of Lloyd's formula can in principle be done on the same energy mesh that is used for the calculation of the charge density [1]. These calculations require to numerically evaluate the derivative of Lloyd's formula. We show that it is possible to accurately determine the derivative without using additional energy mesh points. This is done by interpolating Lloyd's formula with cubic splines which in turn are used to calculate the derivative. We compare the method to calculations without electronic temperatures and show that the spline interpolation does not lead to a significant accuracy lost.

[1] R. Zeller 2005 J. Phys.: Condens. Matter 17 5367, https://dx.doi.org/10.1088/0953-8984/17/35/005

MM 9.72 Mon 18:30 P1

Fiber composite materials in construction of go-cart. — •Mikhail Brusnikin — Moscow, Russia

Lightweighting any vehicle, especially sports equipment, has always been a pertinent issue, and I aimed to determine how significantly material substitution would affect the mass of the power structure by using modern composite constructions instead of classical steel solutions, with the condition of maintaining the same torsional stiffness as the steel sample.

Fiber composite materials are currently at the forefront of technology in terms of stiffness-to-weight ratio and are sufficiently accessible for my research, which was focused on their application in a sports device such as a go-kart.

The assumptions regarding the weight of the final product, which were proposed at the beginning of the research, turned out to be erroneous. Even in the best-case scenario, the weight reduction of the construction was less than anticipated.

MM 9.73 Mon 18:30 P1

RuNNer 2.0: An Efficient and Modular Program for High-Dimensional Neural Network Potentials — •Alexander L. M. Knoll[1,2], Moritz R. Schäfer[1,2], K. Nikolas Lausch[1,2], Moritz Gubler[3], Jonas A. Finkler[3], Alea Miako Tokita[1,2], Gunnar Schmitz[1,2], Henry Wang[1,2], Richard Springborn[1,2], Marco Eckhoff[4], and Jörg Behler[1,2] — [1]Theoretische Chemie II, Ruhr-Universität Bochum, Germany — [2]Research Center Chemical Sciences and Sustainability, Research Alliance Ruhr, Germany — [3]Department of Physics, Universität Basel, Switzerland — [4]Laboratorium für Physikalische Chemie, ETH Zürich, Switzerland

Machine learning potentials (MLPs) have become an important tool for atomistic simulations in chemistry and materials science. As methods in this domain grow increasingly complex and mature, the creation of efficient and user-friendly libraries now receives a lot of attention. We introduce the second major release of RuNNer, an open-source, standalone software package designed for constructing and evaluating second-, third-, and fourth-generation high-dimensional neural network potentials (HDNNPs). RuNNer 2.0 integrates the entire workflow into a fully OpenMP- and MPI-parallel program: from generating atomistic descriptors, via training a specific machine learning model, to its application in molecular dynamics simulations.

MM 9.74 Mon 18:30 P1

Hybrid soldering: Interfacial flux-doping of Cobalt nanoparticles hindering the formation and growth of intermetallic compound (IMCs) layers — •Farzad Khodabakhshi[1,2], Irina Wodak[1], Andriy Yakymovych[1], Gerhard Wilde[2], and Golta Khatibi[1] — [1]Vienna University of Technology — [2]University of Münster

The study investigated hybrid nanocomposite soldering of copper components using a lead-free tin-based solder alloy (Sn-3.5 wt% Ag). To suppress the growth of intermetallic compound (IMC) layers, specifically Cu3Sn and Cu6Sn5, at the interface between the solder alloy and the copper substrate during reflow solidification, a modified flux containing cobalt nanoparticles was applied. The research focused on the effects of incorporating cobalt nanoparticles in different fractions, up to 1.0 wt%, on the microstructural development of the soldered joints and the formation of IMC layers. Additionally, the impact of post-soldering aging treatment, conducted at approximately 180°C for extended periods (up to around 20 days), was assessed. The study analyzed how the alloying of cobalt nanoparticles affected the structure of Cu3Sn and Cu6Sn5 IMC layers, as well as the Sn-based solder alloy. This was done using energy-dispersive X-ray spectroscopy (EDS) elemental mapping in conjunction with field emission-scanning electron microscopy (FE-SEM). Furthermore, the microstructural evolutions of the soldered joints, influenced by the contribution of Co-nanoparticles and the aging treatment, were characterized and discussed using electron channeling contrast imaging (ECCI) microscopy.

MM 10: Topical Talk: M. Salvalaglio

Time: Tuesday 9:30–10:00 Location: H10

Topical Talk MM 10.1 Tue 9:30 H10

Understanding the impact of disconnection flow on microstructure evolution — •Marco Salvalaglio — TU Dresden, Dresden 01062, Germany

In polycrystals, which are composed of misoriented grains and grain boundaries (GBs), microstructure evolution primarily occurs through GB migration. It is widely accepted that GB migration is mediated by the flow of line defects with both step and dislocation characters, i.e., disconnections. Numerous phenomena associated with grain boundary (GB) motion can, in fact, be linked to disconnection flow. This presentation discusses novel fundamental aspects regarding how disconnection flow affects overall microstructural changes. First, with a continuum (phase field) model of GBs that accounts for disconnections, we demonstrate that the generation of internal stress (shear coupling) is the primary factor responsible for deviations from classical curvature-driven grain growth observed in recent experiments. The relative impact of other factors is also briefly discussed. Second, through atomistic simulations, a Markov chain model analysis, and an experimental proof of concept, we demonstrate that asymmetric GBs exhibit direction-dependent mobilities and unidirectional motion under oscillatory driving forces or cyclic thermal annealing. This behavior can be attributed to the microscopic structure of GBs affecting the nucleation barriers of disconnections. Additionally, our findings suggest that applying oscillatory driving forces and non-equilibrium thermal fluctuations accelerates grain coarsening in microstructures, a conclusion further supported by numerical simulations.

MM 11: Topical Session: Defects of Defects

Time: Tuesday 10:15–13:00 Location: H10

Topical Talk MM 11.1 Tue 10:15 H10

The role of disconnections in the shear-migration coupling of grain boundaries — •Marc Legros[1], Armin Rajabzadeh[1], Romain Gautier[2], Nicolas Combe[1], and Frédéric Mompiou[1] — [1]CEMES-CNRS, 29 rue Jeanne Marvig, 31055, Toulouse, France — [2]UMET, Université de Lille, Cité scientifique, 59655 Villeneuve d'Ascq

Grain-boundary (GB)-based plasticity is an alternative to classical, dislocation-based deformation. It is supposed to play a significant role in nanocrystalline metals (d<100 nm) for example, that contain a large proportion of GBs but virtually no dislocations. Among all the mechanisms potentially able to generate a permanent (plastic) deformation, the dominant one is the so-called shear-migration coupling. Despite a recent increase in simulations studies, its experimental characterization remains very scarce. Aside from experimental obstacles, the problem is very vast as real grain boundaries possess at least 5 degrees of freedom and contains a potentially infinite number of disconnections, a specific defect that combines step and dislocation characters.

Using both in-situ TEM experiments and molecular dynamic simulations (NEB Nudge Elastic Band), we have shown that shear-migration coupling involves the displacement of these disconnections. As dislocations in the crystal, the properties of these disconnections seem to guide the coupling mechanism of migrating grain boundaries. The overarching question becomes whether we should still consider a given GB as a crystalline defect or a network of its own, which mechanical properties (mobility, shear coupling) are governed by its nature or by its defects?

MM 11.2 Tue 10:45 H10

Atomistic simulation of point defects behavior inside grain boundaries — •Sergei Starikov, Matous Mrovec, and Ralf Drautz — Ruhr University Bochum, ICAMS, 44801 Bochum, Germany

The properties of point defects play a key role in the description of many phenomena within grain boundaries (GBs), such as pre-melting or atomic diffusion. Compared to the bulk, point defects inside GB are characterized by low formation energy and high complexity. Thus, the thermodynamic/kinetic properties of GBs strongly depend on the behavior of point defects. To reveal general aspects of this relationship, we studied behavior of vacancies and self-interstitial atoms inside tilt grain boundaries for several metals (Ni, Al, Fe, Nb, Mo and W) using atomistic modeling. The simulations revealed that the self-diffusion along the tilt GBs at low/moderate temperatures is mostly driven by migration of self-interstitial atoms. However, heating leads to a change in the GB diffusion mechanism to a more complex exchange process, not related to specific defects, but similar to atomic diffusion in a liquid. This change is due to the disordering complexion transition of GBs, which also significantly affects GB mobility.

MM 11.3 Tue 11:00 H10

Impact of grain boundary defects on grain boundary diffusion and segregation of Cr in Ni bicrystal — Shraddha Sevlikar[1], Mohan G. Muralikrishna[1], Daniel Gaertner[1], Sergei Starikov[2], Tobias Brink[3], Daniel Scheiber[4], Daria Smirnova[3], Daniel Irmer[5], Bengü Tas[1], Vladimir A. Esin[5,6], Vsevolod I. Razumovskiy[4], Christian H. Liebscher[3,7], Gerhard Wilde[1], and •Sergiy Divinski[1] — [1]Institute of Materials Physics, University of Münster, Germany — [2]ICAMS, RU Bochum, Germany — [3]MPI for Sustainable Materials, Düsseldorf, Germany — [4]Materials Center Leoben Forschung GmbH, Leoben, Austria — [5]Mines Paris, PSL University, Évry, France — [6]Université de Lorraine, CNRS, Nancy, France — [7]RC FEMS, RU Bochum, Germany

Grain boundary diffusion of Cr in a near Sigma-11 Ni bicrystal is measured using the radiotracer technique. Opposite to expectations, two distinct contributions to short-circuit diffusion along the nominally single interface are distinguished and related to the existence of two macroscopic facets with distinct inclinations and, as a result, distinct structures. The segregation factor of Cr in Ni is found to be about unity, which is fully supported by ab initio calculations. Using classical atomistic simulations, Ni grain boundary self-diffusion rates are calculated for the symmetric and asymmetric facets. An accelerated self-diffusion kinetics along the asymmetric facet is observed and attributed to the presence of disconnection-like defects. A heterogeneous mechanisms governing atomic migration across distinct facets is corroborated.

15 min. break

Topical Talk MM 11.4 Tue 11:30 H10

Grain Boundary Spinodals: Faceting Instability and the Role of Junction Energetics — •Fadi Abdeljawad — Lehigh University, Bethlehem, PA, USA 18015

Interfaces greatly influence the physical properties and stability of materials microstructures. Of particular interest in crystalline solids are phenomena that occur due to anisotropic interfacial properties. In polycrystalline aggregates, several experimental observations revealed that an initially flat GB profile may facet into hill-and-valley morphologies with well-defined planes and junctions connecting them. Dislocation-like defects exist at facet junctions, which in general connect GB facets with different atomic structures and interfacial properties. Based on classical atomistic simulations and mesoscale modeling, we examine GB faceting transitions and subsequent facet coarsening dynamics. Our modeling framework accounts for anisotropic interfacial energies, and it incorporates junction energetics and their non-local interactions. The hallmark of our approach is the ability to independently examine the various factors affecting this interfacial instability. Theoretical and computational studies predict the dominant growth morphologies as a function of GB facet junction energies. Furthermore, atomistic and mesoscale simulations show that when accounting for junction energetics GB faceting and subsequent facet coarsening is akin to spinodal decomposition in bulk materials. In broad terms, our work provides an avenue to account for GB structural transitions in models of microstructural evolution.

MM 11.5 Tue 12:00 H10

Defect Phase Diagrams for Grain Boundaries in Mg: Chemical trends at Finite Temperatures — •Prince Mathews[1], Rebecca Janisch[2], Tilmann Hickel[1,3], and Jörg Neugebauer[1] — [1]Max-Planck-Institut für Nachhaltige Materialien GmbH, Düsseldorf — [2]Interdisciplinary Centre for Advanced Materials Simulation, Ruhr Universität Bochum — [3]Federal Institute for Materials Research and Testing (BAM), Berlin

Lattice defects are known to directly influence the behaviour of materials. The framework of defect phase diagrams (DPDs) offers a powerful and knowledge-based approach for the tailored design of materials by controlling defect phases in competition to bulk phases. Using ab-initio methods and automized workflows, the DPD for the example of Ga segregation to $\Sigma 7$ [0001] 21.78° (sym. plane 12-30) Mg grain boundary is calculated. It predicts a series of defect phase transformations, which turn out to be in good agreement with transmission electron microscopy experiments. Similar to bulk phases, the stabilities of defect phases can change with temperature. Therefore, different approaches to extend the DPD considering the relevant entropy contributions are discussed. A new sub-lattice model, which is focused on the statistics of grain boundary site column coverages, provides promising insights into temperature-dependent processes of defect phase transformations.

MM 11.6 Tue 12:15 H10

A computationally highly efficient analytical model for the description of defect phase diagrams — •Jing Yang, Mira Todorova, and Jörg Neugebauer — Max Planck Institute for Sustainable Materials, Düsseldorf, D-40237, Germany

In this work, we propose an analytical thermodynamic model for constructing defect and surface phase diagrams. The model is capable of accurately describing the composition-temperature dependence of phase transitions on the surface, including order-disorder ones. It provides a promising alternative to the sublattice model, which is commonly used in the CALPHAD framework to describe solution phases with ordering, as we demonstrate using the system of Mg surface with Ca substitutions. First, as a foundational reference we construct the surface phase transition with grand-canonical Monte Carlo simulation coupled with cluster expansion. The system undergoes a transition from a solid solution (disordered) phase at high temperature, Ca-poor condition to an ordered defect phase with 1/3 Ca coverage. We then show that it is possible to accurately reproduce the critical transition condition with an analytical model assuming a Boltzmann distribution of the phase fractions. Finally, we compare our method with the sublattice model. The proposed method provides a computationally highly efficient and easy-to-parametrize analytical model for constructing defect phase diagrams.

Topical Talk MM 11.7 Tue 12:30 H10

Atomistic structure of fcc-fcc interface in pure iron and in nanomultilayers: insight from atommistic modeling — •Helene Zapolsky[1], Gilles Demange[2], Yuri Borges Gomes Lima[3], Anastasiai Titova[4], and Renaud Patte[5] — [1]GPM, UMR 6634 University of Rouen, France — [2]GPM, UMR 6634 University of Rouen, France — [3]GPM, UMR 6634 University of Rouen, France — [4]GPM, UMR 6634 University of Rouen, France — [5]GPM, UMR 6634 University of Rouen, France

Very great interest in the structure of interphase interfaces between fcc and bcc crystals has historically arisen due to their technological importance in steels. These interfaces also play a crucial role in metallic nanomultilayers (NMLs), where the presence of numerous semi-coherent interfaces leads to a broad spectrum of novel and remarkable properties. One such system, the Cu/Mo NML, holds promise for thermal management applications due to the combination of copper's excellent thermal conductivity and molybdenum's low coefficient of thermal expansion. In these systems, defects at the fcc/bcc interface have a profound impact the thermal properties of the materials. Recently, the Quasiparticle Approach (QA), based on the phase-field methodology, has emerged as a powerful computational tool for modeling and predicting the atomic-scale structure of various interfaces. In this work, we employ atomistic modeling to examine the detailed structure of the fcc/bcc interface, exploring the relationship between this structure and the mode of interface propagation during displacive phase transformations in pure iron and in Cu/Mo NML.

MM 12: Materials for the Storage and Conversion of Energy

Non-Lithiumbased Materials, Characterisation and Simulation Methods

Time: Tuesday 10:15–13:00 Location: H22

MM 12.1 Tue 10:15 H22

Where Electrons Rest After Dark: Polaron Stability in Opto-Ionic 2D Niobium Titanate — •Christoph Dähn[1], Yang Wang[2], Risov Das[2], Bettina V. Lotsch[2], Karsten Reuter[1], and Christian Carbogno[1] — [1]Fritz-Haber-Institut der MPG, Berlin — [2]MPI für Festkörperforschung, Stuttgart

Two-dimensional Niobium Titanate in alkaline solution is promising for opto-ionic energy applications, since it can store photo-generated charge carriers over macroscopic time scales. Although experiments suggest polarons to play a key role for charge storage, identifying the atomistic and electronic mechanisms active in this material has so far proved challenging, also due to the intrinsic disorder of this compound. In this work, we shed light on these aspects by performing hybrid density-functional theory calculations. In a first step, we explore the vast amount of possible lattice decorations resulting from the partial occupation of Ti-sites with Nb, from which we identify a representative set of stable configurations for this disordered material. In a second step, we investigate the stability of polarons at different lattice sites in these configurations. To qualitatively rationalize these results, a fuzzy classification scheme [1] is applied to group comparable polarons according to their local environment. This allows us to analyze how the local environment influences polaron stability and, in turn, long-term charge retention and its underlying mechanisms [2].

[1] K. C. Lai *et al.*, *J. Chem. Phys.* **159**, 024129 (2023).

[2] Y. Wang *et al.*, *J. Am. Chem. Soc.* **146**, 25467(2024).

MM 12.2 Tue 10:30 H22

Beyond Ion Dynamics: Efficient Charge Transport Simulations including Polarons at Battery Scales — •Matteo Rinaldi, Karsten Reuter, and Christian Carbogno — Fritz-Haber-Institut der MPG, Berlin

Polarons have long been recognized as fundamental for charge transport in battery materials - be it as charge carrier or as ion-transport enhancer [1]. Nonetheless, a quantitative modeling of polaron dynamics in such materials has, so far, remained elusive. On the one hand, the activated dynamics of polarons requires time and length scales that are inaccessible with first-principles methods. On the other hand, (machine learned) interatomic potentials do not capture electronic charge transport by construction. In this work, we overcome this hurdle by exploiting force-field models that explicitly account for the electronic viz. polaronic degrees of freedom in a semi-classical, adiabatic fashion. We demonstrate the viability of the approach for lithium titanium oxide (LTO), a prototypical anode material for which polaron hopping is known to play a decisive role [1]. To this end, we train an equivariant message-passing model to density-functional theory data obtained with hybrid functionals. By then performing large-scale molecular-dynamics simulations with this force-field, we investigate both ionic and polaronic transport in LTO as well as their dynamic coupling. We show that polarons diffuse orders of magnitude faster than ions and discuss the implications for the design of battery materials.

[1]M. Kick, C. Scheurer, and H. Oberhofer, ACS Appl. Energy Mater. 4, 8583 (2021).

MM 12.3 Tue 10:45 H22

Tuning electronic structure of CoNi LDHs via surface Fe doping for achieving effective oxygen evolution reaction — •Yunli Shi[1,2], Huaping Zhao[1], Junqi Li[2], and Yong Lei[1] — [1]Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany — [2]School of Materials Science and Engineering, Shaanxi University of Science and Technology, Xian 710021, China

Cobalt and nickel-based layered double hydroxides (LDHs) are promising oxygen evolution reaction (OER) catalysts, but their performance is limited by poor conductivity and low intrinsic catalytic activity. In this study, CoNi LDHs were used as a matrix, with iron sites introduced onto the surface via cation replacement (Fe-CoNi LDHs). Unlike ternary Fe-CoNi LDHs synthesized through conventional one-step methods, the iron sites in Fe-CoNi LDHs are primarily located on the surface and edges of nanosheets, ensuring abundant exposure of reactive sites. Surface doping was found to optimize the coordination environment and electronic structure, reducing the binding energy between reactants and active sites. As a result, Fe-CoNi LDHs exhibit an overpotential of only 260 mV at 10 mA cm-2, demonstrating superior OER performance. This study elucidates the electronic structure and mechanism of enhanced activity, highlighting the potential of surface doping to advance electrocatalytic applications.

MM 12.4 Tue 11:00 H22

Ferromagnetic chiral hybrid organic-inorganic perovskites — •Muskan Nabi and Alessandro Stroppa — CNR - Institute for SuPerconductors, INnovative materials, and devices Italy

In recent years, chiral hybrid organic-inorganic perovskites where the organic cations are the *source* of chirality, have received great attention from the physics and chemistry community. Their functional properties enable the control of light, charge, and electron spins in the same materials. Here, we discuss the intriguing *chirality transfer mechanism* in newly synthesized ferromagnetic chiral hybrid inorganic perovskite and their interplay with magnetism. Although the organic cations are chiral and polar molecules, their arrangement in the crystal structure results in a chiral non-polar space-group P212121. Moreover, we discuss a new chirality order parameter such as the electronic chirality measure (ECM) aiming at quantify the molecular cation chirality taking into account ionic and electronic degrees of freedoms simultaneously. Also, the relation of ECM to physical properties of chiral hybrid perovskites will be discussed.

MM 12.5 Tue 11:15 H22

Enhanced Supercapacitor Performance of Sr-Doped Barium Stannate (BaSnO3) Nanostructures: Synthesis, Characterization, and Electrochemical Insights — Alaa Farid[1,2], •Diaa EL-Rahman Rayan[1,3], Moataz Fayed[4], Saad Mohamed[4], Abdel Hakim Kandil[2], Mohamed Abd El-Nasser[2], and Mohamed Rashad[1] — [1]Central Metallurgical Research and Development Institute (CMRDI), P.O. Box: 87 Helwan, 11421, Egypt — [2]Chemistry Department, Faculty of Science, Helwan University, Cairo, Egypt — [3]Department of Physics, Deraya University, New Minia, Minya, Egypt — [4]Mining and Metallurgy Engineering Department, Tabbin Institute for Metallurgical Studies, (TIMS), Tabbin, Helwan, Cairo Egypt

This study investigates the structural, morphological, thermal, and electrochemical properties of Sr-doped barium stannate. The annealing of undoped BaSnO3 at various temperatures leads to the formation of cubic BaSnO3 phase predominating at 1100 °C. The increasing Sr ion doping induces lattice strain, with slight shifts in the (110) peak. HR-TEM analysis confirms high crystallinity with a significant reduction in particle size from 125.3 to 22.6 nm due to Sr doping. Electrochemical performance tests in a three-electrode configuration show that Sr doping significantly enhances charge storage capacity, with Ba0.8Sr0.2SnO3 achieving a maximum specific capacitance of 1902 F.g-1 at 1 A.g-1. Additionally, the device demonstrated an impressive energy density of 65.6 Wh.kg-1 at a power density of 1633.54 W.kg-1.

15 min. break

MM 12.6 Tue 11:45 H22

Advanced Electron Energy Loss Spectroscopy techniques in catalyst analysis — •Daniela Ramermann, Michael Poschmann, Christoph Göbel, Wenchao Wan, Elisabeth H. Wolf, Saskia Heumann, Holger Ruland, and Walid Hetaba — Max-Planck-Institut für Chemische Energiekonversion, Mülheim an der Ruhr

Electron energy loss spectroscopy (EELS) is a powerful technique that gives access to the electronic structure of the sample, enabling analysis of elemental composition, chemical bonding and oxidation states. Combined with the high spatial resolution of a scanning transmission electron microscope, detailed analysis of a catalyst can be carried out, to gain knowledge about the structure-function relationship. In addition to spatially resolved oxidation state analysis, accessing spectra at higher energy losses than commonly used was recently reported.

We apply these techniques to investigate the oxidation states of a CuZn-based MeOH catalyst system spatially resolved, using self-measured standards. Furthermore, we give examples of the utilization of EELS at high energy losses on a Co-based ammonia decomposition catalyst.

MM 12.7 Tue 12:00 H22

Rapid Identification of Ion Migration in Solid-State Ion Conductors from Machine-Learning Raman Spectroscopy — Manuel Grumet[1], Takeru Miyagawa[1], Karin S. Thalmann[2], Tomáš Bučko[3,4], •Waldemar Kaiser[1], and David A. Egger[1] — [1]TUM School of Natural Sciences, Technical University of Munich — [2]Institute of Physics, University of Freiburg — [3]Faculty of Natural Sciences, Comenius University of Bratislava — [4]Institute of Inorganic Chemistry, Slovak Academy of Sciences

Raman spectroscopy is a rapid, non-invasive, and widely available technique that provides a fingerprint of atomic vibrations within solid-state materials. In this work, we demonstrate evidence of Raman signatures that arise from the migration of ions within solid-state ion conductors. We use a rapid computational framework, which consists of machine-learning molecular dynamics simulations [1] and machine-learned polarizability tensors [2], to predict finite-temperature Raman spectra of two classes of superionic conductors, i.e. AgI [3] and Na_3PnS_4 (Pn=P,Sb) [4]. Our simulation results indicate pronounced and broad low-energy Raman intensities due to the host lattice that are correlated with the diffusion of cations. These insights can open novel synergies with experiments to rapidly screen novel compounds for future battery materials. [1] Miyagawa, et al. J. Mater. Chem. A. 12, 11344-11361 (2024) [2] Grumet, et al. J. Phys. Chem. C, 128, 15, 6464-6470 (2024) [3] Brenner, et al. Phys. Rev. Mater. 4, 115402 (2020) [4] Brenner, et al. J. Phys. Chem. Lett. 13, 25, 5938-5945 (2022)

MM 12.8 Tue 12:15 H22

Ion Dynamics in Li-Garnet Electrolytes from Machine-Learning Molecular Dynamics and Raman Spectroscopy — •Takeru Miyagawa[1], Hyunwon Chu[2], Willis O'Leary[2], Manuel Grumet[1], Jennifer L.M. Rupp[1,2], Waldemar Kaiser[1], and David A. Egger[1] — [1]TUM School of Natural Sciences, Technical University of Munich — [2]Department of Materials Science and Engineering, Massachusetts Institute of Technology

Lithium lanthanum zirconate (LLZO) is a promising electrolyte compound for solid-state batteries. Despite subtle differences in the structural properties, its cubic phase, often stabilized by doping, strongly exceeds the tetragonal counterpart in its ionic conductivity. Here, we study the interplay of Li ion migration and host lattice dynamics in tetragonal and cubic LLZO, and compare the ion dynamics to Ta-doped LLZO, using machine-learning molecular dynamics benchmarked in our previous study [1]. We observe a strongly correlated Li-ion migration in the undoped cubic LLZO at increased temperatures, whereas the tetragonal phase showed no Li ion conduction. In contrast, Li ion hopping is the dominant mechanism in Ta-doped cubic LLZO. Additionally, we compute finite-temperature Raman spectra [2] of the LLZO materials and correlate them to experiments. Our predicted Raman results accurately align with measured Raman spectra, allowing us to reveal concrete vibrational motifs that may be utilized to screen LLZO films for the presence of the conductive cubic phase. [1] Miyagawa, et al. J. Mater. Chem. A 12, 11344 (2024) [2] Thomas, et al. Phys. Chem. Chem. Phys. 15, 6608-6622 (2013)

MM 12.9 Tue 12:30 H22

Extracting Gibbs free energies from local composition fluctuations in atom probe data — •Parisha Diwan, Jianshu Zheng, Rüya Duran, Guido Schmitz, and Sebastian M. Eich — University of Sttugart

In this work, thermodynamic fluctuation theory which is traditionally used for liquids has been extended to solids by incorporating an additional elastic work component to account for local composition variations, which is not present in liquids. In solids, composition fluctuations are quantified through the relative variance of the composition histogram, which is influenced by the evaluation volume size and interface effects. These fluctuations are key to determining the Gibbs free energy of mixing in solid alloys. The technique most suitable for identifying local composition fluctuations is Atom Probe Tomography (APT), which provides high-resolution, 3D spatial chemical information at the atomic level. This allows for the detection of local composition variations in solid materials, making it an ideal tool for the evaluation of the extended fluctuation theory. The study applies this theory to a Cu-Ni alloy, using experimental APT data and spatial frequency distribution analysis. By comparing the results with existing phase diagram data, the method demonstrates its effectiveness in extracting the Gibbs free energy of mixing from local composition fluctuations in solids. The comparison with the latest CALPHAD depiction of the miscibility gap further supports the reliability of the method, showing that the proposed approach can accurately predict thermodynamic properties in solid alloys based on atomic-scale data.

MM 12.10 Tue 12:45 H22

Nanoscopic Bubble Formation during Hydrogen Desorption: Insight from Simulations and Neutron Scattering at the Nanometer Scale and its Impact on Hydrogen Storage Performance — •Arnab Majumdar[1], Neslihan Aslan[1], Martin Müller[1,2], and Sebastian Busch[1] — [1]GEMS at MLZ, Helmholtz-Zentrum Hereon — [2]Kiel University

Chemical hydrogen storage using complex hydrides is promising; characterizing the process at various length scales is crucial for optimizing this approach. At the nanometer length scale and below, neutron scattering is a powerful non-destructive technique, in particular because of hydrogen's significant scattering interaction with neutrons. Additionally, neutrons scatter differently depending on the isotope, allowing deuterium to be used in place of hydrogen.

Small Angle Neutron Scattering (SANS) is suited for characterizing structures at the nanometer length scale. In situ measurements confirmed the occurrence of the hydrogen storage process but the measurements alone could not provide complete details about the processes.

Computer simulations were performed; the most suitable model described the nanoscopic structure using the probability distribution of different compounds. The evolution of initial to final probability distribution was modelled according to different chemical kinetic models. This approach qualitatively reproduces the experimental data, suggesting the presence of trapped gas at the nanometer scale during desorption. This key insight enables an estimate of volumetric performance at the engineering scale, which shows a good match with experiments.

MM 13: Topical Session: Defects of Defects

Time: Tuesday 14:00–15:30 Location: H10

Topical Talk MM 13.1 Tue 14:00 H10

Dynamics of dislocations and grain boundaries during recrystallization of metal nanoparticles — •Eugen Rabkin and Jonathan Zimmerman — Department of Materials Science and Engineering, Technion - Israel Institute of Technology, Haifa, Israel

Recrystallization of bulk metals plays a central role in materials processing, yet it has not been utilized so far for the synthesis of metal nanoparticles. In this work we describe the kinetics of recrystallization and related annealing phenomena in Pt nanoparticles. We uniaxially deformed the particles, annealed them both in-situ and ex-situ, and characterized their morphology and microstructure. Our findings reveal that new grains often nucleate within the parent particle, only to be rapidly reabsorbed back into it, with a strong correlation between this phenomenon and particle size. We propose a model that combines recrystallization and recovery through dislocation annihilation at the particle surface, predicting a critical size for recrystallization in nanoparticles. Finally, we propose a set of rules for nanoparticle recrystallization, mirroring the rules of recrystallization in bulk materials.

MM 13.2 Tue 14:30 H10

Hierarchy of defects in near-$\Sigma5$ tilt grain boundaries in copper studied by length-scale bridging electron microscopy — •Hui Ding[1], Anoosheh Akbari[2], Enze Chen[3], Harald Rösner[2], Timofey Frolov[4], Sergiy Divinski[2], Gerhard Wilde[2], and Christian H. Liebscher[5] — [1]Max Planck Institute for Sustainable Materials, Düsseldorf, Germany — [2]University of M\"unster, Institute of Materials Physics, Münster, Germany — [3]Department of Materials Science and Engineering, Stanford University, Stanford, CA 94305, USA — [4]{Materials Science Division, Lawrence Livermore National Laboratory, Livermore, CA 94550, USA — [5]Faculty of Physics and Astronomy, Ruhr University Bochum, Bochum, Germany

Grain boundaries (GBs) are material imperfections that significantly impact material properties. In this study, we utilized aberration-corrected scanning transmission electron microscopy to examine the structure of a series of near- $\Sigma5(310)[001]$ tilt grain boundaries in copper. Globally, the GB appears flat with no noticeable defects. On the atomic-scale, however, various types of GB defects are observed. When a slight deviation in the misorientation is introduced, a patterning emerges featuring characteristic structural units from the $\Sigma5$ (310) [001] and $\Sigma5$ (210) [001] tilt boundaries. The structural landscape of the GB becomes more complex when GB plane inclination is also present, such as a wavy morphology or staircase-like architecture. Our investigation into GB structure, particularly its inherent defects, is a prerequisite towards gaining atomic-scale insights into their potential impact on material properties.

MM 13.3 Tue 14:45 H10

Data-driven modelling of vacancy segregation to grain-boundaries — •Christoph Dösinger, Oliver Renk, and Lorenz Romaner — Montanuniversität Leoben, Department of Materials Science, Roseggerstraße 12, A-8700 Leoben, Austria

Both vacancies and grain-boundaries (GB) are important defects in materials. The vacancies can interact with the GBs which might lead to a formation of voids, as a result this might start the formation of pores or cracks. From atomistic simulations it is known that vacancies can be attracted to GBs, which indeed may act as sinks for the vacancies. However, such simulations, especially if performed using ab-initio, methods can be tedious and costly. In this work we apply machine learning (ML) methods to predict the segregation energies of vacancies to GBs, which give a measure how strongly a vacancy is attracted to specific sites at different GBs. For this ML approach each segregation site is described by its local environment which can be encoded by using for example Steinhardt or SOAP parameters. Together with the site-specific segregation energies a regression model, in our case a Gaussian Process, is trained. Previously we have shown that this approach can be used to predict the segregation of solutes to grain-boundaries. This method for prediction the segregation of vacancies is tested and applied to GBs in tungsten, for which a complete data-set is available for 15 different GBs ($\Sigma3 - \Sigma43$). By using this diverse set of GBs, it will be possible to predict the GB segregation of vacancies for general GBs or polycrystalline materials.

MM 13.4 Tue 15:00 H10

A high-throughput ab initio segregation study of light elements at Ni grain boundaries and their effects on cohesion — •Han Lin Mai[1], Jörg Neugebauer[1], and Tilmann Hickel[2] — [1]Max-Planck-Institut for Nachhaltige Materialien GmbH, Dusseldorf, Germany — [2]Bundesanstalt für Materialforschung und -prüfung, Berlin, Germany

Segregation of alloying/tramp elements to grain boundaries (GBs) can drastically affect the properties of metallic alloys. We present a high-throughput density-functional theory-based study on the segregation of smaller elements, H, B, C, N, O, P, S, in a variety of FCC Ni GBs and their effects on cohesion. To support GB engineering efforts, we investigate the thermodynamics of segregation and calculate its effects on interface cohesion. These elements often play a significant role in engineering alloys, but their positioning at GBs is ambiguous and challenging to study. The study utilizes efficient and highly automated workflows using the integrated development environment pyiron. We discuss chemical and structural trends for segregation and cohesion at GBs for these elements. In order of segregation binding strength at GBs, the trend is approximately $O > B, S > P > N = C = H$. Elemental trends for maximum segregation binding strength across various GB models are largely consistent, enabling qualitative cross-element comparisons through small GB sets. However, conventional metrics, such as GB energy, are insufficient for predicting segregation strength or quantity for these elements.

MM 13.5 Tue 15:15 H10

Mechanistic Influence of Interstitial Solutes on Hydrogen Trapping at $\Sigma5$ GB in γ-Fe — •Poulami Chakraborty, Mauricio Rincon Bonilla, and Elena Akhmatskaya — Basque Centre for Applied Mathematics, Bilbao, Spain

The local variation of grain boundary atomic structures and chemistry caused by segregation of impurities influences the macroscopic properties of polycrystalline materials. Here, the effect of co-segregation of carbon and boron on hydrogen segregation at a $\Sigma 5$ (210) [001] tilt grain boundary in γ-Fe phase is studied by density functional theory. The grain boundary structure predominantly features kite-like motifs, which are disrupted by atomic-scale defects. First-principles calculations indicate that carbon and boron exhibit the strongest segregation tendency. Their interaction with aluminum is notably repulsive, leading to aluminum depletion at the grain boundary. Subsequently, the effect of boron and carbon co-segregation is studied with the introduction of H at the GB. Our comprehensive investigation provides valuable insight in the interaction of interstitial impurities with substitutional solutes, which, strongly influences grain boundary composition and the properties of the interface.

MM 14: Materials for the Storage and Conversion of Energy (joint session MM/KFM)

Time: Tuesday 14:00–15:15 Location: H22

MM 14.1 Tue 14:00 H22

Multiscale defective interfaces for realizing Na-CO2 batteries with ultralong lifespan — •changfan xu, tzuchin huang, and yong lei — Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany

The cycling capability of Na-CO2 batteries has been impeded by limitations in the kinetics of cathodic CO2 reduction/evolution reaction (CO2RR/CO2ER) as well as the challenging process of depositing/stripping metallic Na during cycling.[1-3] Herein, a ”two-in-one” electrode with multiscale defective FeCu interfaces (CP@FeCu) is presented, improving the kinetics of CO2RR/CO2ER and modulating sodium deposition behavior.[4] The enhancement of sodiophilicity and catalytic properties is attributed to multiscale defective FeCu interfaces, as revealed by experimental and theoretical investigations. The defect and valence oscillation effects originate in multiscale defective FeCu interfaces, effectively facilitating reactant adsorption and Na2CO3 decomposition during CO2RR/CO2ER processes, along with exceptional cycling stability of 2400 cycles (4800 h) at 5 μA cm*2. Meanwhile, the CP@FeCu with high sodium affinity creates a uniform electric field and strong Na adsorption, promoting favorable nucleation sites for dendrite-resistant and durable anodes. This work provides scientific insights into the design of ”two-in-one” electrodes, which are crucial for addressing challenges in sodium anodes and CO2 cathodes. [1] Small 2023, 2206445 [2] Adv. Funct. Mater. 2023, 2300926 [3] Energy Environ. Mater. 2024, 7, e12626 [4] Adv. Mater. 2024, 2409533

MM 14.2 Tue 14:15 H22

Electro-chemo-mechanical behavior of a layered cathode material upon cycling — •Robert Löser[1], Yug Joshi[2], Roham Talei[1], and Guido Schmitz[1] — [1]University of Stuttgart, Stuttgart, Germany — [2]Max-Planck-Institut für Nachhaltige Materialien GmbH, Düsseldorf, Germany

The mechanical properties of lithium-ion cathode materials play a critical role in determining battery performance such as cycle life, durability, and safety, especially when the battery is under external pressure which is typical for all-solid-state batteries. This research investigates LiCoO2 (LCO), a prevalent hexagonal layer-structured cathode material, and explores its mechanical responses during de-/lithiation using sputter-deposited thin films and nanoindentation. The values of the experimental Young*s modulus in pure (101) and (003) lattice orientations are quantified to 337.1 * 8.7 GPa and 267.9 * 7.2 GPa, respectively, in the fully lithiated state. Furthermore, a substantial texture-dependent decrease in Young*s modulus upon lithium deintercalation is demonstrated, probably due to modification of the bonding interactions between the cobalt oxide layers. Delithiation also elevates the relative contribution of plastic deformation, indicating that dislocation glide becomes easier in deintercalated states. By extensive cycling, the Young*s modulus in higher lithiated charge-states decreases considerably which is most-likely due to irreversibility of phase transitions. The work provides valuable insight on the dynamic changes of the mechanical properties during electrochemical cycling of LiCoO2, which paves the way for all other layered cathode materials.

MM 14.3 Tue 14:30 H22

MnTiO$_3$ as a Carbon-Free Cathode for Rechargeable Li-oxygen Batteries — Doaa Ahmed[1,2], Wernfried Mayr-Schmölzer[1], Mustafa Çelik[3,4], Abdulkadir Kizilaslan[3,4], and •Gregor Vonbun-Feldbauer[1,2] — [1]Institute of Advanced Ceramics, TU Hamburg, Germany — [2]Institute of Soft Matter Modeling, TU Hamburg, Germany — [3]Research, Development and Application Center (SARGEM), Sakarya University, Turkey — [4]Department of Metallurgical and Materials Engineering, Engineering Faculty, Sakarya University, Turkey

Lithium-oxygen batteries (LOB) are promising energy storage systems due to their high theoretical energy density. However, their main challenges are the sluggish kinetics of oxygen reduction and evolution reactions (ORR/OER) and high charge overpotentials. To overcome these challenges, the development of a suitable catalyst is crucial. Here, MnTiO$_3$ was investigated as a carbon-free cathode catalyst using density functional theory (DFT) calculations and experimental approaches. DFT calculations revealed the coexistence of Mn and Ti energy levels near the Fermi level of MnTiO$_3$, which facilitates ORR/OER. This feature endows MnTiO3 with a bifunctional role in promoting battery performance. Our DFT-based investigation further elucidates the surface stability and catalytic properties of MnTiO$_3$. In addition, experiments confirm that the electrochemical reactions on MnTiO$_3$ follow a two-electron pathway. LOBs with MnTiO$_3$ exhibit a total overpotential of 1.18 V and 1.55 V from DFT and electrochemical measurements, respectively, and current densities up to 1 A/g.

MM 14.4 Tue 14:45 H22

Modeling and optical characterization of Lithium deposition on Copper current collectors — •Len Kimms[1], Tjark Ingber[2], Diddo Diddens[1,2], and Andreas Heuer[1] — [1]Institut für physikalische Chemie, Universität Münster — [2]Helmholtz Institute Münster (IEK-12), Forschungszentrum Jülich GmbH

In this contribution, we will present modeling results of the initial deposition of lithium metal on a copper current collector combined with experimental insights. Zero–excess lithium–metal batteries (ZELMBs) may offer higher energy densities, better safety, and reduced cost by reducing the amount of lithium employed in the cell. Instead of an excess of lithium as electrode, the anode is formed in situ during charging. When charging the battery, lithium is plated on the current collector directly. However, the lifespan of ZELBMs in practical applications is still limited by irreversible loss of active lithium. The loss is induced by the high reactivity of lithium which causes parasitic side reactions and dendrite growth during charging cycles. To uncover the mechanisms at play, the initial deposition of lithium metal has been experimentally investigated by plating varying amounts on a copper surface with different current densities. The deposits have been characterized by scanning electron microscopy (SEM) and laser scanning microscopy (LSM) in an automated way. Numerical simulations of a simple geometric model were employed to uncover the relevant mechanisms which govern the growth over different stages. Combining the experimental and numerical results, an effective description of the deposition has been found.

MM 14.5 Tue 15:00 H22

Preparation of Prussian blue analogue materials and their application to potassium-ion batteries — •Ping Hong, Huaping Zhao, and Yong Lei — Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany

Prussian blue (PB) and its analogs (PBAs), with their unique open framework structure and chemical stability, have emerged as promising cathode materials for potassium-ion batteries (PIBs). PB and PBAs feature three-dimensional channels, facilitating rapid potassium-ion intercalation and de-intercalation, thus delivering excellent rate performance. Furthermore, its low-cost synthesis and environmentally friendly properties provide a strong foundation for potential commercial applications. Despite these advantages, the practical application of PBAs is hindered by challenges such as their high solubility in electrolytes and limited cycle stability and life. To overcome these limitations, we optimized synthesis techniques (by simple adjustment of the co-precipitation method) and structural design, leading to significant improvements in material performance. In addition, a series of adjustments were made to the binder, electrolyte, and voltage range used in the batteries. The improved PBA cathode exhibited remarkable cycling stability, showing almost no capacity decay after 500 cycles at a current density of 100 mA/g within the voltage range of 2.0-4.0 V. It maintained excellent cycling performance even under high current conditions, providing strong support for the advancement of high-performance PIBs.

MM 15: Invited Talk: C. Scheu

Time: Wednesday 9:30–10:00 Location: H10

Invited Talk MM 15.1 Wed 9:30 H10

Grain Boundary Defect Phases in Thermoelectric Materials: Impact on physical properties — •Christina Scheu[1], Ruben Bueno Villoro[1], Siyuan Zhang[1], Baptiste Gault[1], Duncan Zavanelli[2], and Gerald Jeffrey Snyder[2] — [1]Max-Planck-Institute for Sustainable Materials, Max-Planck-Str. 1, 40627 Düsseldorf, Germany — [2]Northwestern University, Clark Street 633, 60208, Evanston, USA

Grain boundary defect phases are known since more than three decades, but mostly the impact on mechanical properties was investigated. In our work we were able to correlate the atomic structure and chemical composition of grain boundary defect phases in different thermoelectric materials to the electrical and thermal properties. For example, we were able to show by atom probe tomography and scanning transmission electron microscopy that grain boundaries in p-type Ti(Co,Fe)Sb Half-Heusler thermoelectric materials possess a significant Fe segregation and Co depletion compared to the bulk. Atomic column resolved scanning transmission electron microscopy images reveal that the grain boundary phase has a hexagonal close packed stacking compared to the face centered cubic stacking of the bulk with lattice distances differing from those of any known bulk phase. The grain boundary defect phase acts as fast charge carrier pathway providing a high electrical conductivity while simultaneously reducing the thermal conduc

MM 16: Topical Session: Thermophysical Properties of Bulk Metallic Glasses and Bulk Metallic Glass-forming Liquids

Time: Wednesday 10:15–13:00 Location: H10

Topical Talk MM 16.1 Wed 10:15 H10

Microstructure and transport in model isotropic amorphous solids — •Peter Derlet — Condensed Matter Theory Group, Paul Scherrer Institut, Switzerland

Amorphous solids lack long range order, however structural heterogeneity can exist over intermediate length scales suggesting the notion of a glassy microstructure. Such spatial variations, whatever they may be, can also be related to variations in thermally driven structural fluctuation time scales. In this talk, I will present atomistic simulations of model isotropic (metallic) binary glass systems spanning the microsecond timescale, and discuss the resulting amorphous structure in terms of bond frustration, demonstrating that despite the strong disorder, a percolative region containing strong medium range order emerges that fundamentally affects transport and dissipation. Particular focus will be given to how such simulations can give insight into experiments probing arrested colloidal glasses obtained through isotropic compression, and structural decorrelation in a metallic glass probed by long-time x-ray photon correlation measurements.

MM 16.2 Wed 10:45 H10

Liquid-like versus Stress-Driven Dynamics in a Metallic Glass Former Observed by Temperature Scanning XPCS — •Maximilian Frey[1], Ralf Busch[1], and Eloi Pineda[2] — [1]Chair of Metallic Materials, Saarland University, Campus C6.3, 66123 Saarbrücken, Germany — [2]Department of Physics, Institute of Energy Technologies, Universitat Politècnica de Catalunya - BarcelonaTech, 08019 Barcelona, Spain

Using high flux synchrotron radiation (ESRF, ID10), we study a Pt-based metallic glass former via X-ray photon correlation spectroscopy (XPCS) upon temperature scanning through the glass, glass transition and supercooled liquid (SCL). In the equilibrium SCL, the obtained intensity autocorrelation functions are well-described by a conventional Kohlrausch-William-Watts (KWW) model. Yet, in the glass and especially the glass transition region, this approach fails. Instead, we demonstrate that a multiplication of two KWW functions allows to describe the complex decay shape. Within the glass transition region, the fit parameters of the two separate KWW fits decouple massively. While one KWW component models the compressed shape of glass-typical non-equilibrium dynamics, the other fit maintains stretched liquid-like characteristics. We demonstrate that the compressed decay can be likely addressed to ballistic-like atomic motions while the stretched component apparently reflects (sub-)diffusive atomic motions, which are both superimposed in the non-equilibrium.

MM 16.3 Wed 11:00 H10

Non-monotonic hydrodynamic relaxations in a nanochannel — •Linnea Heitmeier[1,2], Thomas Voigtmann[1,2], and Jesper Schmidt Hansen[3] — [1]Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt (DLR), Köln, 51170 — [2]Heinrich Heine University, Universitätsstraße 1, Düsseldorf — [3]DNRF Center Glass and Time, IMFUFA, Department of Science, Systems and Models, Roskilde University, DK-4000 Roskilde

Nanotechnology is an active research field with applications in the everyday-life, electronics and medicine.

In my talk, I will present results of Molecular-Dynamics Simulations of a glass-forming liquid, which is confined in a nanochannel and excited with a sinusoidal force in order to probe the velocity relaxation on different lengthscales.

I show that the velocity relaxation behavior in different regions of the channel depends non-monotonically on the position of the fluid.

To explain the results, I will make use of the Maxwell-model for fluids, which states that a fluid behaves like an elastic solid on small timescales and like a viscous fluid on large timescales.

The simulation results can be recovered by this model, when using generalizations of this model:

On the one hand, a two-mode-Maxwell-model captures the contributions from the short-time dynamics and the slow structural relaxation to the viscosity. On the other hand, a spatially non-local generalization of the Maxwell-model allows to capture the velocity relaxation in the channel depending on different positions.

MM 16.4 Wed 11:15 H10

Structural Complexity and Atomic-Scale Dynamics in Metallic Glasses — •Emel Gurbuz and Elif Ertekin — University of Illinois Urbana-Champaign

Metallic glasses (MG) become prominent for their exceptional mechanical strength, corrosion resistance, and versatile processing capabilities, all strongly linked to their amorphous atomic structures. Despite extensive research, the interplay between structural motifs, their connectivity, and the resulting dynamic behavior during glass formation remains insufficiently understood.

This study uses molecular dynamics simulations to explore the dynamics of glass formation in MG systems with varying compositions (Fe_xZr_{100-x}, Co_xZr_{100-x}, Cu_xZr_{100-x}). By analyzing melt-quench trajectories, we identify key structural motifs, such as five-fold icosahedra, and examine their role in the "freezing in" process. Regions with rapid solidification and liquid-like behavior are characterized by tracking atomic diffusivity distributions over time. Remarkably, sequences of connected icosahedra persist as liquid-like regions even at low temperatures, facilitating ionic transport.

Our findings reveal critical insights into the mechanisms governing structural and dynamic complexity in MGs, advancing the understanding of their formation and potential for designing functionally optimized materials.

15 min. break

Topical Talk MM 16.5 Wed 11:45 H10

Structural relaxation and deformation of bulk metallic glasses — •Gerhard Wilde — Institute of Materials Physics, University of Münster, Germany

In metallic glasses, relaxation is discussed in the context of shear transformation zones, viscous flow, structural medium-range order (MRO) and even crystal nucleation. However, the structural origin of different relaxation modes and how these structures change during relaxation, rejuvenation or deformation is rather unclear. In order to address some of these related aspects, calorimetric measurements have been performed together with TEM-based analyses of the local medium range order structures before and after plastic deformation as well as after controlled thermal relaxation. The combined results of macroscopically averaging and spatially resolved analyses are discussed with respect of the correlations between relaxation, deformation and modifications of the MRO structure.

MM 16.6 Wed 12:15 H10

Tracing the Roots of Elastic Heterogeneity in Metallic Glass — •Reza Rashidi[1,2], Birte Riechers[1], and Robert Maass[1,2,3] — [1]Federal Institute of Materials Research and Testing (BAM), Unter den Eichen 87, 12205 Berlin, Germany — [2]Department of Materials Engineering, Technical University of Munich, 85748 Garchingen, Germany — [3]Department of Materials Science and Engineering, University of Illinois at Urbana-Champaign, Urbana, IL 61801, USA

Metallic glasses (MGs) show structural and temporal heterogeneities over a broad range of time and length scales. With the aid of atomistic simulations, we can explain these dynamic and structural fluctuations at the nanometer scale. Here, our focus shifts to the larger length scale of property variations and the ongoing exploration of their origin. In past work, we suggested that cooling constraints during solidification could lead to elastic heterogeneities and therefor an elastic microstructure on the scale of ~100 nm (Materials & Design 229 (2023) 111929). In this presentation, we further support this idea by examining various casting geometries and thermal histories, tracking how elastic decorrelation lengths change with sample size and position within the MG. We also find that thermal annealing reduces decorrelation length-scale gradients and smooths out fluctuations in modulus values (Scripta Materialia 255 (2025)116380). In concert with the nano-elastic property assessment, we leverage spatially-resolved scanning nanobeam diffraction in the search for a structural origin of elastic microstructure.

MM 16.7 Wed 12:30 H10

Yield surfaces of glass-forming fluids — •Stephan Domann[1,2] and Thomas Voigtmann[1,2] — [1]Institut für Materialphysik im Weltraum, DLR Köln — [2]Heinrich-Heine-Universität

The yielding of amorphous solids depends in principle on the geometry of the deformation applied to the solid. This defines a "static" yield surface in the state of principal stresses that is typically described by empirical models (such as von Mises, Tresca, Drucker-Prager etc). In a similar vein, approaching the glass transition from the fluid side, the flow stresses approach a dynamical yield stress, defining the dynamical yield surface as the geometry of the flow is varied. Owing to the difficulty of imposing arbitrary steady deformation geometries, both experiment and simulation data are scarce.

We will discuss an approach to model yield surfaces that is rooted in a first-principle theory originally developed by Fuchs and Cates, the combination of mode-coupling theory of the glass transition with the integration-through transients framework (ITT-MCT). Using suitable simplifications, we recover some of the well-known empirical yield surface descriptions as limiting cases. It also sheds light on the qualitative differences arising between models of the upper-convected and the lower-convected type. We also performed non-equilibrium molecular-dynamics simulations of a model glass former to determine the dynamical yield surface. Surprisingly, this attains a shape that is in qualitative agreement with the lower-convected model, although common expectation is that upper-convected models are more canonical in emerging from microscopic descriptions of glass forming fluids.

MM 16.8 Wed 12:45 H10

Unveiling the Asymmetry in Density within the Shear Bands of Metallic Glasses — •Harald Rösner[1], Arabinda Bera[2], and Alessio Zaccone[2] — [1]Universität Münster, Institut für Materialphysik, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany — [2]University of Milan, Department of Physics "A. Pontremoli", via Celoria 16, 20133 Milan, Italy

Plastic deformation in metallic glasses at room temperature leads to the development of shear bands due to shear localization. In many experiments, shear bands have shown local density variations along their path, with a distinct imbalance in magnitude between local densification and dilation. However, a comprehensive mechanistic understanding or theory to explain this asymmetry has been lacking until now. Here, we introduce a new model [1] that consists of a sequential arrangement of alternating topological charges, generating a dipolar field. The resulting microscopic displacement field, when integrated into the deformation gradient tensor, provides an accurate analytical solution for the observed imbalances in the density variations. The implications of this model are discussed, highlighting the potential to elucidate a broader range of observations in shear bands.

[1] H. Rösner, A. Bera, and A. Zaccone, Phys. Rev. B, 110(1), 014107 (2024).

MM 17: Development of Calculation Methods

Machine Learning, DFT

Time: Wednesday 10:15–12:45 Location: H22

MM 17.1 Wed 10:15 H22

Premature Convergence, It's Nothing to be Embarrassed About: Solving Performance Issues with Swarm-Based Global Optimization to Generate Pt Nanoparticle Ensembles — •Julian Holland[1], Malgorzata Makos[3], Difan Zhang[4], Mal-Soon Lee[3], Roger Rousseau[3], Chris-Kriton Skylaris[2], and Vanda Glezakou[3] — [1]Fritz-Haber-Institut der MPG, Berlin — [2]University of Southampton, Southampton, UK — [3]Oak Ridge National Laboratory, Oak Ridge, USA — [4]Pacific Northwest National Laboratory, Three Cities, USA

Swarm-based global optimisation (GO) algorithms have proven successful in exploring potential energy surfaces (PESs) of chemical systems. However, they are often limited by their serial implementation. Our GO software, pyGlobOpt, uses an asynchronously parallel artificial bee colony (ABC) methodology, mitigating this limitation. We enhance pyGlobOpt further by tuning parameters against a new, general, ensemble generation assessment criterion. Using this criterion, we were also able to demonstrate how to overcome premature convergence, an issue pervading the use of the ABC algorithm for some systems, using a clustering-based methodology. We demonstrate that using the clustering algorithm alongside tuned pyGlobOpt parameters can lead to a 5-fold increase in the number of unique low-energy structures found as well as more than halving the average energetic distance from the global minimum. We produce ensembles of thermodynamically relevant Pt nanoparticles with varying hydrogenation using our enhanced software and compare to experimental results.

MM 17.2 Wed 10:30 H22

Charge Equilibration in Machine Learning Potentials — •Martin Vondrak[1,2], Johannes Margraf[1], and Karsten Reuter[2] — [1]Bayreuth University, Bayreuth, Germany — [2]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

Machine learning (ML) techniques have recently been shown to bridge the gap between accurate first-principles methods and computationally cheap empirical potentials. This is achieved by learning a mapping between a system's structure and its physical properties. To this end, state-of-the-art models typically represent chemical structures in terms of local atomic environments. This inevitably leads to the neglect of long-range interactions (most prominently electrostatics) and non-local phenomena (e.g. charge transfer), resulting in significant errors in the description of e.g. polar molecules or materials in non-isotropic environments. To overcome these issues, we are developing ML frameworks for predicting charge distributions in molecules based on Charge Equilibration (QEq). Here, atomic charges are derived from a physical model using environment-dependent atomic electronegativities. In this presentation, we will demonstrate strategies for creating long-range interatomic potentials on the example of Kernel Charge Equilibration (kQEq) models combined with local Gaussian Approximation Potentials (GAP). An alternative approach, incorporating QEq into the equivariant MACE neural network scheme will also be discussed.

MM 17.3 Wed 10:45 H22

Development of on-the-fly kinetic Monte Carlo framework with neural network potentials for surface chemistry — •Tomoko Yokaichiya, Tatsushi Ikeda, Koki Muraoka, and Akira Nakayama — The University of Tokyo, Tokyo, Japan

It is established that adsorbate-adsorbate lateral interactions in heterogeneous catalysis significantly influence adsorption and activation energies. To further our understanding of the degree to which such lateral interactions affect catalytic properties, we develop an "on-the-fly" adaptive kinetic Monte Carlo (kMC) simulation scheme. The scheme proceeds by energetically evaluating each configuration, including its local adsorbate-rich environment, using a neural-network potential then stores them to a database for efficient reuse in later kMC iterations. We apply this scheme to the industry-relevant interactions of H adsorption and diffusion on Pd and Pt surfaces as well as CO oxidation on Pt surfaces. With this scheme, we are able to elicit the extent lateral adsorbate-adsorbate interactions influence surface reactions and diffusion.

MM 17.4 Wed 11:00 H22

DECAF: An Open Source Local Atomic Environment Classifier — •King Chun Lai, Sebastian Matera, Christoph Scheurer, and Karsten Reuter — Fritz-Haber-Institut der MPG, Berlin

Classification of local atomic environments (LAEs) is an inevitable task in most atomic-scale modeling and simulation. The reason is trivial, atoms' characteristics are predominantly determined by neighbors within a limited radius. The task itself, however, is abstract and error-prone due to the diversity of structures and the often ambiguous relationship between geometry and atomic behaviors. To address these issues, we have developed the open-source package DECAF during the last years [1]. DECAF automatically identifies equivalence groups within atomic structure datasets on the basis of the LAEs. We showcase the usage of the DECAF package on a set of nanotructures. We explain the theoretical background as well as the influence of different options to control the outcome. A particular feature is DECAF's ability for out-of-sample classification, identifying LAEs that differ from any groups in the training set. We provide examples where this has been exploited such as automatic process exploration [2] or active learning.

[1] Lai *et al.*, J. Chem. Phys **159**, 024129 (2023). DOI: 10.1063/5.0160369 Available: https://gitlab.mpcdf.mpg.de/klai/decaf
[2] Lai *et al.*, ChemRxiv (2024). DOI: 10.26434/chemrxiv-2024-jbzr7

MM 17.5 Wed 11:15 H22

Accurate TDDFT Excited-State Spectra Across the Full Spectral Range — •Matthias Kick and Troy Van Voorhis — Massachusetts Institute of Technology, Cambridge, MA, USA

Theoretically, electronic excitations can be obtained by analyzing the frequency components of the time-dependent dipole moment obtained from real-time time-dependent density functional theory (RT-TDDFT) simulations. Yet, an exact treatment of electronic excitations in large systems with TDDFT is computational prohibitive. Super-resolution techniques such as compressed sensing typically fail due to the presence of a quasi-continuum of electronic excitations. We present a new approach where we combine exact short-time dynamics with approximate frequency space methods. As a prototypical test system, we use an organic dye-molecule adsorbed on a semi-conductor quantum-dot surface. We calculate the entire electronic absorption spectrum of this system and find that our approach can accurately capture narrow features and a quasi-continuum of states at the same time. We see a reduction of the required amount of data points up to a factor of 20 compared to standard Fourier analysis. By doing so, our method allows us to study electronic properties of large systems in ways that are not currently possible.

15 min. break

MM 17.6 Wed 11:45 H22

Beyond-DFT Machine-Learning Interatomic Potentials and Applications to Covalent-Organic Frameworks — •Yuji Ikeda, Axel Forslund, and Blazej Grabowski — University of Stuttgart, Germany

Covalent-organic frameworks (COFs) are nanoporous crystalline materials composed of covalent organic secondary building units (SBUs), primarily composed of light elements such as C, N, O, and H. Many COFs exhibit a quasi-two-dimensional layered structure, stabilized by van der Waals (vdW) interactions. Machine-learning interatomic potentials (MLIPs) offer an exciting opportunity to explore COFs, enabling access to extended time and length scales in molecular dynamics (MD) simulations. To accurately model vdW interactions, MLIPs must be trained on datasets that include these effects, often derived from vdW-DFT functionals. However, vdW-DFT methods are essentially semi-empirical, with parameters calibrated for experimental agreement, raising concerns about their transferability. Instead, we propose generating training data from post-Hartree-Fock methods, such as coupled-cluster (CC) calculations, which are non-empirical and provide beyond-DFT accuracy. By utilizing MLIPs trained on these high-accuracy datasets, we aim to investigate the structural properties of COFs in unprecedented detail.

MM 17.7 Wed 12:00 H22

Performance and limits of finite-temperature DFT for SiO2 — •Axel Forslund, Jong Hyun Jung, Blazej Grabowski, and Yuji Ikeda — Institute for Materials Science, University of Stuttgart, Germany

Silicon dioxide (SiO2) is a widely studied compound, yet far from fully understood. It exists in a variety of different phases, several of which are dynamically stabilized. These structures require dynamic vibrations of the atoms to not transform, and pose a challenge from an atomistic modeling point of view. Even in recent publications where state-of-the-art machine-learning interatomic potentials (MLIPs) have been used, the predictions differ significantly from experiments. For example, the transition between the two dynamically stabilized phases beta-quartz and cristobalite is very sensitive, and a single meV/atom shift can change the transition by 100 K. Not only the accuracy of the MLIP and the method for free-energy calculations matters, but also the underlying ab initio data play a crucial role. We demonstrate this sensitivity, and provide a simplified, yet precise method of estimating the quartz-cristobalite transition temperature. This approach is accurate enough to closely estimate the transition temperature using new density-functional-theory (DFT) functionals, and we demonstrate this for several functionals and on-top corrections. Our method is also efficient enough for using the random-phase approximation (RPA), which provides a transition temperature in very good agreement with the average CALPHAD value, and thus serves as a benchmark for the development of improved DFT functionals.

MM 17.8 Wed 12:15 H22

DSKO: Dancing through DFTB Parametrization — •Artem Samtsevych, Yihua Song, Christoph Scheurer, Karsten Reuter, and Chiara Panosetti — Fritz Haber Institute of the Max Planck Society, Berlin, Germany

Density Functional Tight-Binding (DFTB) offers a computationally efficient alternative to *ab initio* methods, bridging between the accuracy of DFT and the speed of semiempirical models. The approximate nature of DFTB makes its reliability highly dependent on parameter quality. While recent advancements have significantly improved the parametrization of the so-called repulsive potential, the parametrization of the so-called electronic part of the DFTB interaction remains relatively simplistic and underdeveloped.

Here, we present our in-house DFTB Slater-Koster Optimizer (`DSKO`), a novel DFTB parametrization framework that aims at producing highly accurate and transferable electronic parameter sets, under rigorous physical constraints. By incorporating robust optimization algorithms and physics-informed loss functions, `DSKO` generates parameters that align well with high-level DFT references, particularly in predicting electronic properties like density of states (DOS) and band gaps. The versatility of `DSKO` facilitates the application of DFTB to a wide spectrum of materials science challenges, from catalysis to energy storage, paving the way for routine high-fidelity semiempirical simulations.

MM 17.9 Wed 12:30 H22

A Fundamental Study of Slater-Koster Tables in Density Functional Tight-binding within Trial Nickel Oxides Systems — •Yihua Song, Artem Samtsevich, Christoph Scheurer, Karsten Reuter, and Chiara Panosetti — Fritz Haber Institut

Density-Functional Tight Binding (DFTB), a semiempirical approximation to Density Functional Theory (DFT), is widely used thanks to its undoubtful computational efficiency, which allows to access large scale systems out of reach for DFT, while keeping adequate accuracy and direct electronic structure information. To be mentioned, even with non-spin polarized and non +U reference, the optimized parameters are able to be highly transferable to spin-polarized, DFTB+U and large scale calculations without any pain. The speed advantage in DFTB originates from precalculating distance dependent two-center interaction integrals for each atomic species pair, following the Slater-Koster (SK) principle[1]. In a fundamental study of the prototypical system Ni/NiOx, we test the hypothesis of adapting the SK integrals depending on the local environment. Considering a trial structure containing Ni in different oxidation states simultaneously, we find that assigning to each Ni "type" its optimal SK parametrization significantly improves the description of the band structure and density of states. Generalizing this concept opens a promising way towards adaptive, reliable, machine-learnable SK parameters.

MM 18: SYMD contributed

Time: Wednesday 10:15–13:15 Location: H23

MM 18.1 Wed 10:15 H23

Relation Between Element Specific Chemistry and Basis Set Size of Machine Learned Interatomic Potentials — •Haitham Gaafer, Jan Janssen, and Joerg Neugebauer — Max Planck Institute for Sustainable Materials, Düsseldorf, Germany

Machine learned interatomic potentials (MLIP) have gained popularity in materials science for their scalability and accuracy on par with the Density Functional Theory (DFT) training data. Based on the linear scaling with the number of neighbors, the primary focus in the recent years was increasing the flexibility of MLIPs to further improve their accuracy, as demonstrated by approaches such as Neural Network potentials and the Atomic Cluster Expansion (ACE). The Bessel functions and Chebyshev polynomials gained popularity as basis sets to represent the atomic bonds and orbitals. Nonetheless, the connection between an MLIP's basis set and its capability to represent the chemical complexity of various elements is not yet well understood.

In this study, we use ACE, as implemented in the Pacemaker software package, to investigate three non-magnetic transition metals (i.e., Al, Au, and Cu). For each element, we parameterize computationally efficient ACE potentials based on a minimal basis set to achieve a given root-mean-square error (RMSE) across both training and testing datasets. We find that the complexity of the MLIP primarily depends on the scaling of the per-atom energy distribution rather than the chemical complexity of the elements. Consequently, it is primarily a numerical effect rather than a chemical effect.

MM 18.2 Wed 10:30 H23

Physics-Based Generative Models: Enhanced Structure-Property Sampling in Inverse Materials Design — •Patricia König[1], Nicolas Bergmann[1], Piero Coronica[2], Chiara Panosetti[1], Hanna Türk[1], Karsten Reuter[1], and Christoph Scheurer[1] — [1]Fritz-Haber-Institut der MPG, Berlin — [2]Max Planck Computational and Data Facility, Munich

Data-driven approaches for the inverse design of novel materials with desired properties have become a key tool in materials discovery. Here, we introduce a framework using physics-based Generative Adversarial Networks for enhanced structure-property sampling via latent space design.

We are interested in sampling structures of two chemical systems associated with different relevant physical quantities, like the work function in the electrochemical adsorption of iodide and hydroxide on copper surfaces, and the oxygen chemical potential in the CO to CO_2 conversion over an amorphous RuO_2 catalyst. As part of our framework, we track and evaluate the structural diversity and convergence of our generator with machine-learning interatomic potentials and quantitative metrics. This enables a high throughput and cost-effective evaluation of structural guesses and their related properties to leverage the full potential of generative models. Concluding, we are showing on two model systems how to explore a vast chemical space of datasets with sparse areas, particularly structures with high free energies in transition states and diverse amorphous surface structures, thereby advancing the understanding and design of novel materials.

MM 18.3 Wed 10:45 H23

Active learning-based automated construction of Hamiltonian for structural phase transitions: a case study on $BaTiO_3$ — •Mian Dai[1], Yixuan Zhang[1], Nuno Fortunato[1], Peng Chen[2], and Hongbin Zhang[1] — [1]Institute of Materials Science, Technical University of Darmstadt, Darmstadt 64287, Germany — [2]Physics Department and Institute for Nanoscience and Engineering, University of Arkansas, Fayetteville, Arkansas 72701, USA

The effective Hamiltonians have been widely applied to simulate the phase transitions in polarizable materials, with coefficients obtained by fitting to accurate first-principles calculations. However, it is tedious to generate distorted structures with symmetry constraints, in particular when high-ordered terms are considered. In this work, we implement and apply a Bayesian optimization-based approach to sample the potential energy surface, automating the Hamiltonian construction by selecting distorted structures via active learning. Taking $BaTiO_3$ (BTO) as an example, we demonstrate that the Hamiltonian can be obtained using fewer than 30 distorted structures. Follow-up Monte Carlo simulations can reproduce the structural phase transition temperatures of BTO, comparable to experimental values with an error $<$ 10%. Our approach can be straightforwardly applied on other polarizable materials and paves the way for quantitative atomistic modelling of diffusionless phase transitions.

MM 18.4 Wed 11:00 H23

Comparing linear and deep learning surrogate models of materials electronic structure — •Valdas Vitartas, Chen Qian, James Kermode, and Reinhard Maurer — University of Warwick, Coventry, UK

The self-consistent electronic Hamiltonian matrix from Density Functional Theory (DFT) gives access to the electronic band structure and the density of states of a material, albeit at a large computational cost. Over recent years, several surrogate models based on linear parametrization and deep learning have been proposed to efficiently learn the electronic Hamiltonian as a function of the configuration and composition of materials. In this work, we compare two such models, the ACEhamiltonians [npj Comput. Mater. 8, 158] and MACE-H. Both provide a representation of the Hamiltonian in atomic orbital basis in terms of an equivariant many-body expansion of local atomic environments. In the case of ACEhamiltonians, the model parametrization is linear; for MACE-H, the representation serves as input to a message-passing neural network. The models are trained on reduced, valence-only Hamiltonian matrices for bulk gold and silicon generated from all-electron DFT via an approximately eigenspectrum-conserving transformation. We discuss the inherent strengths and weaknesses of the models by illustrating their accuracy, performance, data efficiency, and their ability to predict electronic quantities of interest for out-of-distribution configurations.

MM 18.5 Wed 11:15 H23

MACE-H: Equivariant Hamiltonian prediction with many-body expansion message passing — •Chen Qian, Valdas Vitartas, James Kermode, and Reinhard J. Maurer — University of Warwick, UK

The machine learning prediction of Kohn-Sham Density Functional Theory (DFT) Hamiltonians has the potential to accelerate the prediction of electronic properties, such as electronic band structures and electron-phonon coupling, while avoiding computationally expensive self-consistent field iterations. We introduce the MACE-H graph neural network, which combines the MACE body-order expansion message passing scheme with node-degree expansion blocks to efficiently generate messages that incorporate all relevant SO(3) irreducible representations. This model achieves high accuracy and high computational efficiency in capturing the local chemical environment. We demonstrate the model performance using several open materials benchmark datasets for 2D materials, achieving sub-meV prediction errors on matrix elements. Moreover, we discuss how the many-body expansion achieves higher data efficiency and examine its effect on out-of-distribution prediction for nanostructures featuring long-range interactions. To assess prediction outputs, we analyze the correlation between errors and hermiticity. The high computational efficiency and accuracy make the model a good candidate for electronic structure prediction in large-scale systems and high-throughput material screening.

15 min. break

MM 18.6 Wed 11:45 H23

Inferring Structure-Property Relationships with Artificial Intelligence: A Lignin Case Study — •Matthias Stosiek and Patrick Rinke — Technical University Munich, Munich, Germany

The potential of lignin as an abundant, underutilized biopolymer is increasingly being realized. A key challenge for the targeted production of lignins remains the poorly understood relation between lignin properties and its complex structure. Artificial intelligence (AI) methods could reveal such structure-function relationships but remain elusive in biomaterials research.

Structurally diverse lignins are extracted from birch wood combining the Aqua Solv Omni (AqSO) biorefinery process and AI-guided data acquisition[1]. Each lignin sample is characterized with 2D nuclear magnetic resonance (NMR) spectroscopy. A total of 95 collected NMR spectra are complemented with measurements of key lignin properties such as the antioxidant activity.

To establish structure-function relationships, we first correlate regions of the NMR spectra with the corresponding property measurements. Subsequently, we use RFR feature importance analysis to identify structural features that correlate with each property and provide a chemical interpretation of our findings. For instance, we find that a higher number of β-O-4 bonds leads to a lower surface tension in water indicating a more linear lignin structure. Our structure-inference approach is designed to be general and applicable to a wide range of materials and characterization data.

[1] D. Diment et al., ChemSusChem 2024, e202401711.

MM 18.7 Wed 12:00 H23

Machine learning electrostatics: Open challenges from batteries to proteins — •Max Veit — Technische Universität Darmstadt, DE

Long-range interactions such as electrostatics have long been a concern in developing accurate, efficient machine learning potential energy surfaces (ML-PES). Such potentials have now become established as a powerful technique allowing simulations of complex structures and processes with unprecedented realism and accuracy. However, the most widespread and successful methods to date do not incorporate any interactions beyond a fixed cutoff range, typically a few coordination shells. First, we need to ask the question of how methods with such an obvious limitation can be so successful, even applied to systems where long-range electrostatic interactions are known to be relevant. Second, we need to ask what approach, among the many proposed over the last decade or so, is the most appropriate if we want to incorporate long-range interactions in an accurate, efficient, and physically appropriate way. We investigate these questions in the context of a technologically relevant, experimentally accessible test system: lithium-intercalated graphite or nearly-graphitic nanoporous carbon. We first discuss the characteristics of this system that make it uniquely suited to machine learning simulation, then turn to the difficulties involved in defining what exactly makes a “good” electrostatic model, or long-range model in general, in the context of machine learning potentials, and finally discuss the implications for other systems – such as complex biomolecules – just out of the current reach of ML-PES simulations.

MM 18.8 Wed 12:15 H23

Data driven prediction of relative stability of binary and ternary TCP phases. — •Mariano Forti, Ralf Drautz, and Thomas Hammerschmidt — Interdisciplinary centre for advanced materials simulation, Ruhr-University Bochum

The study of precipitation of topological close packed(TCP) phases is of primary importance for the performance of superalloys. However, the structural complexity of these intermetallic compounds and the chemical complexity of the superalloys with typically up to ten elements hampers the exhaustive sampling of chemical space by density-functional theory (DFT) calculations. We overcome the related computational limitations by combining machine learning (ML) techniques with descriptors of the local atomic environment of the TCP phases and the use of interatomic potentials to predict phase properties with high precision. We illustrate our methodology studying the relative stability of the complex phases R, P, M and δ in binary and ternary systems produced from the main components in Co, Ni and Fe based superalloys.

MM 18.9 Wed 12:30 H23

Inverse Materials Design with Large Language Models — •Jan Janssen and Joerg Neugebauer — MPI for Sustainable Materials, Düsseldorf, Germany

Large language models (LLM) are trained on a vast amount of scientific literature to learn the included semantic, conceptional, and statistical relationships. The LLM applies these relationships to generate responses in natural language based on the context of the conversation. This raises the question: Can a LLM replace a scientist? Or how does the thought process of a scientist differ from the statistical approach of the LLM? Can the LLM make us better scientists?

We benchmark the capabilities of current LLMs to design new materials using atomistic simulations. While the required Python programming is challenging for the LLM and suffers from hallucination, this can be addressed with an agent-based approach by providing the LLM with a series of simulation workflows for the pyiron workflow framework. With these simulation workflows the LLM is not only capable to calculate material properties but can also invert the process and leverage statistical models to identify alloying compositions which match a pre-defined materials property, enabling inverse materials design.

Our benchmarks highlight the importance of developing scientific workflows. The more a workflow reduces the technical and scientific complexity of studying a given materials property the easier it is to use for LLMs and scientists alike. In this way LLMs also help us as scientists to validate and improve our scientific workflows. https://github.com/jan-janssen/LangSim

MM 18.10 Wed 12:45 H23

Workflow Utilities within the NOMAD Infrastructure: Lowering the Barrier to FAIR Data Management for Computational Materials Science — •J.F. Rudzinski[1], E. Boydas[1], N. Daelman[1], B. Mohr[1], J.M. Pizarro[1], T. Bereau[2], C. Draxl[1], L.M. Ghiringhelli[3], M. Girard[4], D. Usvyat[5], R. Valenti[6], and S. Botti[7] — [1]CSMB, HU Berlin — [2]ITP, Heidelberg Uni. — [3]Dept. of Mater. Sci. and Eng., FAU Erlangen — [4]Max Planck Inst. for Poly. Res., Mainz — [5]Inst. für Chem., HU Berlin — [6]Inst. für Theor. Phys., GU Frankfurt/M — [7]RC-FEMS, Ruhr Uni. Bochum

NOMAD [nomad-lab.eu] [1] is an open-source, community-driven data infrastructure, focusing on materials science data. The NOMAD software can automatically extract data from the output of over 60 simulation codes, has been extensively expanded to support advanced many-body calculations and classical molecular dynamics simulations, and allows straightforward specialization via a rapidly developing plugin-based ecosystem. Both standardized and custom complex simulation workflows not only streamline data provenance and analysis but also facilitate the curation of AI-ready datasets. This contribution will focus on recently developed workflow functionalities and utilities within the NOMAD infrastructure. These advances enable highthroughput interfacing with the NOMAD repository, opening improved discovery pipelines by leveraging the benefits of NOMAD’s comprehensive and FAIR-compliant data management system [2].

[1] Scheidgen, M. *et al.*, JOSS **8**, 5388 (2023).
[2] Scheffler, M. *et al.*, Nature **604**, 635-642 (2022).

MM 18.11 Wed 13:00 H23

Freedom of design: towards in silico design of molecules with desired quantum-mechanical properties — •Leonardo Medrano Sandonas[1], Alessio Fallani[2], Julian Cremer[3], Alexandre Tkatchenko[2], and Gianaurelio Cuniberti[1] — [1]TUD

Dresden University of Technology, Germany. — [2]University of Luxembourg, Luxembourg. — [3]Pfizer Worldwide R&D, Germany.

The rational in silico design of chemical compounds requires a deep understanding of both the structure-property and property-property relationships that exist across chemical compound space (CCS), as well as efficient methodologies for defining an inverse property-to-structure mapping. In this presentation, we will discuss these relationships in the CCS sector spanned by small [Sci. Data 8, 43 (2021)] and large [Sci. Data 11, 742 (2024)] drug-like molecules, highlighting the existence of the "Freedom of design" principle [Chem. Sci. 14, 10702 (2023)]. The insights gained are subsequently leveraged to design molecules with desired properties. To this end, we first developed a variational autoencoder (VAE) approach and demonstrated that CCS can be parameterized using a finite set of quantum-mechanical (QM) properties [Nat. Commun. 15, 6061 (2024)]. We showcased the capabilities of this method by conditionally generating de novo molecular structures, interpolating transition paths for chemical reactions, and providing insightful insights into property-structure relationships. We expect our work will contribute to the development of advanced generative frameworks that enhance the in silico design and identification of molecules for specific chemical processes.

MM 19: Invited Talk: L. Bourgeois

Time: Wednesday 15:00–15:30 Location: H10

Invited Talk MM 19.1 Wed 15:00 H10

Structure, interfacial segregation and transformations of solid-state precipitates in aluminium alloys — •Laure Bourgeois[1,2], Nikhil Medhekar[2], and Matthew Weyland[1,2] — [1]Monash Centre for Electron Microscopy, Monash University, Victoria, Australia — [2]Department of Materials Science and Engineering, Monash University, Victoria, Australia

Solid-state precipitates are key components of many materials, and none more so perhaps than of lightweight alloys such as aluminium. These precipitates are often deeply buried inside the alloy matrix due to having at least one dimension at the nanoscale or even sub-nanoscale. These precipitates are also, in most cases, metastable phases that do not exist in a monolithic state, thus constituting difficult objects to characterise at the atomic scale. In this contribution we present the structural determination of several precipitate phases in lightweight alloys, including the classic Al-Cu, Al-Au and Al-Ag systems. Using a combination of scanning transmission electron microscopy and atomistic simulations, we reveal the existence of new interfacial structures and precipitate phases, and propose atomic-scale models for the mechanisms of nucleation and growth. This includes unexpected pathways for the formation of desired strengthening precipitates. These insights are used as a starting point to predict the precipitation behaviour of other, largely unexplored, alloy systems.

MM 20: Topical Session: Thermophysical Properties of Bulk Metallic Glasses and Bulk Metallic Glass-forming Liquids

Time: Wednesday 15:45–18:30 Location: H10

Topical Talk MM 20.1 Wed 15:45 H10

Magnetic properties of Fe-based amorphous alloys produced by melt-spinning and selective laser melting — •Paola Tiberto — INRIM, Torino, Italy

Amorphous soft-magnetic materials play an important role as core constituents in improving the energy transformation efficiency of electrical machines and passive electrical components. Although the melt-spinning process remains the main technique for obtaining amorphous soft-magnetic ribbons with remarkable soft magnetic properties, new and efficient production methods based on additive manufacturing have been developed in recent years, enabling the direct synthesis of larger elements. Ribbons were obtained by a conventional melt-spinning process while 3D-printed samples were produced by additive manufacturing via Selective Laser Melting (SLM) using powder of the same alloy as a precursor. In this study, we investigate the hysteresis properties of amorphous Fe-Si-B-based alloys in ribbon shape and 3D-printed bulk samples produced by different casting techniques. The SLM processing conditions have been observed to play a crucial role in the microstructure of the printed parts and, therefore, in their magnetic properties, due to their dependence on morphology. The effect of different printing parameters on magnetic properties, such as laser power and scan speed, has been studied. This study highlights the critical link between microstructure engineering through manufacturing techniques and the resulting magnetic performance, offering insights into optimizing both for enhanced energy efficiency in magneto-electrical applications.

MM 20.2 Wed 16:15 H10

Advancements in Developing Fe-Based Metallic Glasses for Additive Manufacturing of Soft Magnetic Components — •Amirhossein Ghavimi[1], Maryam Rahimi Chegeni[1], Purbasha Sharangi[2], Uma Rajput[2], Gabriele Barrera[2], Enzo Ferrara[2], Paola Tiberto[2], Isabella Gallino[3], and Ralf Busch[1] — [1]Saarland University, Chair of Metallic Materials, Campus C6.3, 66123 Saarbrücken, Germany — [2]INRIM, Strade delle Cacce 91, Torino, Italy — [3]Department of Materials Science and Engineering, Metallic Materials, TU-Berlin, Ernst-Reuter-Platz 1, 10587 Berlin, Germany

This research aims to create suitable Fe-based soft-magnetic amorphous alloys for the 3D printing of motor components. Since a fully amorphous structure of the 3D-printed parts is expected to improve motor efficiency, i.e. increase magnetic softness and decrease energy losses, the glass-forming ability (GFA) is enhanced through the judicious change of the alloy chemical composition while maintaining competitive soft magnetic properties. The GFA of the compositions was studied by evaluating the critical casting thickness (dc) of the samples. Subsequently, XRD, DSC and DTA were used to characterize the structure and thermal behavior of the samples. The magnetic properties were determined by means of VSM in addition to the evaluation of losses. The eutectic zone of the Fe-Si-B system was experimentally determined. Evaluation of quaternary and quinary component alloys involved studying the effects of promising elements such as phosphorous and nickel on GFA and magnetic properties.

MM 20.3 Wed 16:30 H10

Ni-Nb-(Ta)-P-Based Bulk Metallic Glasses: The Origin of Glass Formation Based on Thermodynamics, Kinetics, Structure and Crystallization Behavior — •Lucas M. Ruschel and Ralf Busch — Chair of Metallic Materials, Saarland University, 66123, Saarbrücken, Germany

Ni-Nb-based bulk glass-forming alloys are among the most promising amorphous metals for industrial applications due to their incomparable combination of strength, hardness, elasticity and plasticity. A successful approach in alloy development is so-called minor alloying, where metallic glasses with improved properties and enhanced GFA are produced, if the proper minor alloying element is chosen for the respective base alloy. Here, minor additions of P to the binary Ni-Nb system increase the GFA up to a record value of 5 mm, which surpasses the binary $Ni_{62}Nb_{38}$ alloy by 150 %. The partial substitution of Nb by Ta further boosts the GFA up to 6 mm. To elucidate the origins of the significant improvement in GFA, key properties such as the thermodynamics and kinetics of the system are studied, including the driving force for crystallization and the kinetic slowdown of viscosity during the transition from the equilibrium liquid to the glassy state. The primary precipitating phase, critical for glass formation, is identified by high-energy synchrotron X-ray diffraction (HEXRD) under containerless electrostatic levitation conditions. Complementary low-temperature HEXRD experiments reveal the structural evolution across a wide temperature range, offering a comprehensive understanding of the mechanisms responsible for the enhanced GFA.

MM 20.4 Wed 16:45 H10

Mechanical Behavior of Phase-Separated Zr-Al-Fe-Y Metallic Glasses for Prospective Implant Applications — •Devinder Singh[1,2], Parthiban Ramasamy[1], Anna Sophie Jelinek[3], Christoph Gammer[1], Zaoli Zhang[1], and Jürgen Eckert[1,3] — [1]Erich Schmid Institute of Materials Science, Austrian Academy of Sciences, Jahnstraße 12, 8700, Leoben, Austria — [2]Amity School of Applied Sciences, Amity University Uttar Pradesh, Lucknow 226028, India — [3]Department of Materials Science, Montanuniversität Leoben, Jahnstraße 12, 8700, Leoben, Austria

Phase separation arises from the substitution of Y in Zr70-xAl12.5Fe17.5Yx (x=0-25 at.%) metallic glasses (MGs), resulting in the formation of nano-amorphous domains within a glassy matrix. The glasses with $x > 10$ show a typical liquid phase separation-induced two-glassy phase (Zr-rich and Y-rich) morphology with droplet-like microstructures. Atom probe tomography (APT) analysis confirms the formation of nanometer-sized Y-enriched clusters for x=15 and 20. The micro-hardness and nano-hardness are found to be in the range of 4.58-5.73 GPa and 5.22-6.11 GPa. The Zr-based MGs exhibit Young's moduli in the range of 81-91 GPa, which are lower than that of Co-Cr-Mo, 316L SS and Ti-6Al-4V commercial implant alloys. Evaluation of the cytocompatibility of the MG ribbons reveals high metabolic activity and well-spread human gingival fibroblast (HGF) cells on the surface of x=10 and 15 samples. Thus, the two glassy-phase Zr-based MGs free of toxic elements (Ni and Cu) exhibit suitable mechanical properties and biocompatibility for implant applications.

15 min. break

Topical Talk MM 20.5 Wed 17:15 H10

Diffusion and nucleation in Al-Ni melts using machine-learned MD simulations — Johannes Sandberg[1,2,3], Leon F. Granz[2,3], and •Thomas Voigtmann[2,3] — [1]Universitë Grenoble-Alpes, Grenoble, France — [2]Heinrich-Heine-Universität, Düsseldorf, Germany — [3]Deutsches Zentrum für Luft- und Raumfahrt, Köln, Germany

The microstructure that forms during solidification of metallic melts greatly influences the material properties. It depends crucially on the microscopic transport properties, and the initial phase selection in the cricial nucleus. Simulation of these phenomena faces two contradictory demands: while the relevant length and time scales match well that of classical molecular dynamics simulations, the sensitive dependence on details of the interatomic interactions is only captured in much smaller-scale quantum-mechanical simulations. In recent years, machine-learned interaction potentials have helped to reconcilce these requirements, allowing MD simulations to be performed with almost DFT-like accuracy.

I will present results that we have obtained using high-dimensional neural network potentials (HDNNP) to the case of Al-Ni melts and nucleation processes therein. Crucially, we assess the performance of the HDNNP by comparing to structural and dynamical experimental data of the liquids at different compositions. This reveals also how the level of DFT closure chosen in the quantum-mechanical simulations used to train the network influences the prediction of thermophysical quantities.

MM 20.6 Wed 17:45 H10

Study of solidification behaviour of undercooled Zr-Ni-Cu melts — •Chu Yu[1,4], Fan Yang[2], Dirk Holland-Moritz[2], Yindong Fang[1,4], Ivan Kaban[3], Stephanie Lippmann[4], and Peter K. Galenko[1] — [1]Otto Schott Institute of Material Research, Friedrich Schiller University Jena, Jena, Germany — [2]Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt, Cologne, Germany — [3]Leibniz IFW Dresden, Institute for Complex Materials, Dresden, Germany — [4]Institute of Applied Physics, Friedrich Schiller University Jena, Jena

We investigate the solidification behaviour of the glass-forming $Zr_{50}Cu_{35}Ni_{15}$ alloy employing different levitation techniques. The primary phase solidified from the undercooled melt has been found to be independent of the degree of undercooling up to a level beyond the hypercooling limit, as observed by time-resolved X-ray diffraction. The crystal growth velocity has been measured employing electromagnetic levitation (EML), where solidification occurs under stronger fluid-flow conditions compared to previous studies employing electrostatic levitation (ESL). In both cases the observed growth velocity increases with increasing undercooling, before reaching a plateau at undercoolings between 260-320 K. However, at small undercooling the growth velocities measured with EML are slightly higher than that in ESL. The solidification kinetics is discussed in terms of different crystal growth models, taking into account the effect of fluid flow. The works is supported by DFG, DLR, ESA via MULTIPHAS-project Nr. 50WM1941, and ProChance-exchange Program of the FSU Jena.

Topical Talk MM 20.7 Wed 18:00 H10

The effect of composition on the thermodynamics, structure, mechanical properties and atomic motion of (Pd-Pt)42.5Cu27Ni9.5P21 alloys — •Ralf Busch — Saarland University, Saarbrücken, Germany

According to basic hard sphere models Pt should replace Pd in the Pd42.5Cu27Ni9.5P21 alloy. But Pt42.5Cu27Ni9.5P21 shows significant structural differences compared to the Pd based alloy. To study the differences, we prepared a series of (Pd-Pt)42.5Cu27Ni9.5P21 alloys replacing Pd with Pt. We assess the thermodynamic functions revealing that the driving force for crystallization increases with the increase of the Pt content, which is in line with the decreasing critical casting thickness. The Pt-richer alloys are thermodynamically more fragile than the Pd-rich alloys, which is revealed by a larger specific heat capacity and a faster drop of the configurational entropy in the Pt-richer alloys. High energy XRD (HEXRD) studies reveal that the structure of the Pt rich alloys is dominated by its change in medium range order whereas the Pd-rich alloy is dominated by extraordinary short range order. The mechanical properties change drastically from a ductile behavior on the Pt-rich side to an embrittlement with increasing Pd content and decreasing Pt concentration. Nano-indentation investigations together with the HEXRD studies reveal that the embrittlement with increasing Pd-content can be connected to the structural changes. We used XPCS to study the atomic dynamics of the alloys as a function of temperature and wave vector.

MM 21: Interface Controlled Properties, Nanomaterials and Microstructure Design

Time: Wednesday 15:45–18:30 Location: H22

MM 21.1 Wed 15:45 H22

Plateau-Rayleigh-type failure mode of porous films and interconnects near massive substrates: mitigation strategies — •Gideon Henkelmann[1], Xinyan Wu[2], and Jörg Weissmüller[1,3] — [1]Institute of Materials Physics and Technology, Hamburg University of Technology, Germany — [2]Institute of Optical and Electronic Materials, Hamburg University of Technology, Germany — [3]Institute of Hydrogen Technology, Helmholtz-Zentrum hereon, Geesthacht, Germany

Nanoporous thin films are under study as functional materials for actuation, photonics, catalysis, energy storage and as semiconductor interconnects. However, these thin films tend to self-detach from their substrate. The same failure mode is also observed in sintered silver paste, a widely used electronics interconnect material. In this work, we discuss the origin of the underlying instability. Based on those insights, we derive a mitigation strategy that depends on gradient in porosity. Combining experiment with kinetic Monte Carlo simulation, we validate the strategy and optimize the composition profile. An exponential gradient is found optimum, and this is rationalized by theory. Our approach greatly improves the structural stability of nanoporous thin films, enabling their more reliable use in advanced applications.

MM 21.2 Wed 16:00 H22

Compressive behavior and connecting topology of monolithic nanoporous niobium — •Seoyun Sohn[1,2], Shan Shi[3,1], Jürgen Markmann[1,2], Stefan Alexander Berger[1], and Jörg Weissmüller[2,1] — [1]Institute of Hydrogen Technology, Helmholtz-Zentrum Hereon, 21502 Geesthacht, Germany — [2]Institute of Materials Physics and Technology, Hamburg University of Technology, 21073 Hamburg, Germany — [3]Research Group of Integrated Metallic Nanomaterials Systems, Hamburg University of Technology, 21073 Hamburg, Germany

This study investigates the mechanical behavior of nanoporous (NP) Nb fabricated through liquid-metal dealloying, with an eye on the role of structure size and topology. Results from X-ray nanotomography and macro-compression tests confirm that coarsening degrades yield strength and that Young's modulus deviates from scaling laws previously developed for NP Au made by dealloying in aqueous media. Our analysis reveals that the scaled genus, a measure of network connectivity, of NP Nb observed from the tomographic reconstructions is lower than what has been reported for NP Au. This reduced connectivity provides an obvious explanation for the low modulus of NP Nb. Furthermore, the structural dispersion implies that additional structural descriptors should be acknowledged to account for the mechanical differences between liquid-metal dealloyed materials and those synthesized via conventional aqueous dealloying.

MM 21.3 Wed 16:15 H22

Unravelling the metal-support interaction of sub-monolayer Pt thin films on manganese oxide via photoelectron spectroscopy — •Manuela Arztmann[1], Raul Garcia-Diez[1], Johannes Frisch[1], and Marcus Bär[1,2,3,4] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Germany — [2]Energy Materials In-Situ Laboratory Berlin, Germany — [3]Helmholtz-Institut Erlangen-Nürnberg für Erneuerbare Energien, Germany — [4]Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany

In heterogeneous catalysis, metal-support interactions (MSI) have been shown to greatly influence the selectivity and activity of catalysts, with reducible supports as preeminent examples. The various oxidation states accessible for manganese oxide allow to accommodate different amounts of oxygen vacancies, making it a promising support with tunable properties for catalysis. Studies show that the oxidation state of manganese is closely linked to its promoter capabilities in catalysis, though the MSI is not well understood so far. In this 'in-system' study, the chemical and electronic structure of the interface between Pt and manganese oxide was investigated by XPS/UPS as a function of Pt surface coverage. The thin film model catalysts were prepared by e-beam evaporation in a system directly connected to the XPS/UPS setup, enabling precise control of the Pt thickness from sub-monolayer levels to thick metal-like Pt layers, allowing for a systematic study of the property evolution in the near surface region without leaving vacuum conditions. Our results reveal an enhanced reduction of the manganese oxide with increasing Pt surface coverage indicating significant MSI.

MM 21.4 Wed 16:30 H22

Optical and electrical properties of borophene and borophene/silicon junction — •yaser abdi[1,2], masoud taleb[1], alireza eskandari[2], zahra alavi[2], mohsen moayedi[2], and nahid talebi[1] — [1]Institute of Experimental and Applied Physics, Kiel University, 24118 Kiel, Germany — [2]Department of Physics, University of Tehran, 1439955961 Tehran, Iran

Borophene, a 2D monolayer of boron atoms, possesses unique properties that have led scientists to conclude that it could be an excellent alternative to graphene in future electronic device applications. In this talk, which is based on our recent work on synthesis [1] and characterization [2] of optical [3] and electrical properties of borophene and borophene/silicon Schottky junction, I will discuss about the growth of borophene using a chemical vapor deposition approach and investigation of its optical and electrical behaviors. Leveraging advanced deep-subwavelength cathodoluminescence spectroscopy, we reveal the extreme anisotropic optical response of borophene in the visible range[3]. Finally, direct growth of borophene on silicon to make Schottky junction will be explained and some opto-electrical measurements will be presented. The optoelectronic response of a borophene/silicon-based detector is approximately ten times higher than that of detectors fabricated by transferring 2D materials onto silicon, due to the excellent junction formed by the direct growth of borophene on silicon.

[1] ACS Applied Materials & Interfaces 2021 13 (7), 8844-8850 [2] ACS Applied Nano Materials 2024 7 (11), 13712-13719 [3] arXiv preprint arXiv:2404.13609v2

MM 21.5 Wed 16:45 H22

Atomistic computer simulations of the influence of grain boundary phases on segregation — •Tobias Brink, Dongjin Kim, and Gerhard Dehm — Max Planck Institute for Sustainable Materials, Düsseldorf, Germany

The properties of polycrystalline materials are often strongly affected by grain boundary (GB) segregation. Segregation energies, in turn, strongly depend on the available segregation sites and their atomic environments in the GB. At the atomic level, however, GBs are not only distinguished by their macroscopic, crystallographic parameters: different GB phases (or "complexions") can coexist even along the same GB and consequently affect available segregation sites. Similar as for bulk phases, the equilibrium atomic structure and chemistry of GBs changes based on temperature, pressure, concentration, chemical potential, etc.

Here, we investigate Ag segregation to [111] tilt GBs in Cu with hybrid molecular dynamics/Monte Carlo computer simulations using EAM potentials. These GBs are of interest because they exhibit two GB phases, "pearl" and "domino". Depending on the misorientation, either the pearl or the domino phase can more easily accommodate Ag segregants. As a consequence, the GB phases not only display distinct segregation behavior, but the stability of the GB phases is now also a function of the Ag excess concentration. An outlook on the effects of other segregants will be given and comparisons to experimental results will be discussed.

MM 21.6 Wed 17:00 H22

Characterizing the strength and stability of grain boundaries in Ni alloys by atomistic simulations — Reyhaneh Ghassemizadeh, •Daniel F. Urban, and Christian Elsässer — Fraunhofer Institute for Mechanics of Materials IWM, Freiburg, Germany

When increasing the in-service performance of engineering metallic materials, interfaces such as phase or grain boundaries (GB) may act as the weakest links. For the nickel-base superalloy Alloy 718 intergranular cracking can be a relevant damage mechanism as result of high-temperature fatigue in an oxygen-rich environment. The reliable prediction of the adhesion and mechanical stability of interfaces between two grains in a microstructure of a material from atomistic calculations remains a challenge. A possible approach to systematically address this issue is an idealized cleavage simulation analyzed in terms of the Rose-Ferrante-Smith universal binding energy relationship (UBER) which results in a measure for the ideal work of separation and the maximum tolerable normal strain. With this approach, we analyze the stability of GBs in Alloy 718 using density functional theory calculations and thereby distinguish the influence of the different alloying elements on the strength of these interfaces. Furthermore, we systematically examine the influence of oxygen at the GBs and thereby shed light on the respective segregation-induced embrittlement in polycrystalline Ni systems. Our results can be used to parametrize traction separation laws used in finite element modelling, allowing for microstructure-sensitive modelling of fatigue crack formation and growth.

MM 21.7 Wed 17:15 H22

Ce-doped Ni-based nanocrystal ribbons for Near-Perfect Infrared Absorbers — •Timuçin Emre Tabaru[1], Ali Karatutlu[2], Iremnur Duru[1], and M. Fatih Kilicaslan[3] — [1]Department of Electrical Electronics Engineering, Sivas University of Science and Technology, 58000 Sivas, Turkey — [2]Institute of Materials Science Nanotechnology and National Nanotechnology Research Center (UNAM) Bilkent University Ankara 06800, Türkiye — [3]Department of Engineering Fundamental Sciences, Sivas University of Science and Technology, 58000 Sivas, Turkey

Absorption properties of Ni-based ribbons prepared with a composition of 75 % Ni, 10 % Cr, 8 % Si, 5 % Fe, 2 % B, and %1 Ce-doped were investigated in the infrared region. The ribbons were prepared by melt spinning, and the samples exhibited a nanocrystalline structure due to rapid solidification. The total absorbing effectiveness of the Ni-based ribbons reached a maximum of about %93 at 3-5 *m mid-wave infrared (mid-IR) window when the ribbons were doped with Ce causing an approximate 5% improvement in the mid-IR absorption. Overall, the composite films provide over 80% IR absorption at the wavelengths from 3 *m to 25 *m. Due to the superparamagnetic behavior of the Ni-based composite film suggesting a decrease in electrical conductivity, a high impedance allows such high IR absorption over a large EM spectrum. This indicates that Ce-doped Ni composite film can be a good candidate for thermal emitters and infrared imaging, and for integrating into small-pixel uncooled infrared detectors.

MM 21.8 Wed 17:30 H22

Tracking the emergence and persistence of abnormal grain growth in the commercial aluminum alloy AA5252 using 3D X-ray microscopy — •Helmuth-André Schulz-Harder[1], Jules M. Dake[1], Wolfgang Ludwig[2], Haixing Fang[2], Pierre-Olivier Autran[2], Karolína Gutbrod[1], Markus Ziehmer[1], Madlen Atzen[1], Thomas Wilhelm[3], Volker Schmidt[3], and Carl E. Krill III[1] — [1]Institute of Functional Nanosystems, Ulm University, Germany — [2]The European Synchrotron (ESRF), Grenoble, France — [3]Institute of Stochastics, Ulm University, Germany

The origin of abnormal grain growth (AGG) remains unclear despite decades of investigation, even though this phenomenon has far-reaching implications for a wide range of industrial applications. A significant challenge lies in the scarcity of time-resolved 3D data on AGG. To address this, we acquired a time series of 3D maps of the commercially available aluminum alloy AA5252 using synchrotron-based diffraction-contrast tomography (DCT). The reconstructed grain maps reveal the presence of extreme abnormal grains, the evolution of which could be observed over time and traced back nearly to the point of emergence. To further explore the influence of second-phase particles (known to be present in AA5252) on the growth of abnormal grains, we conducted complementary phase-contrast tomography (PCT) measurements. The combination of these datasets provides new insight into the locations where abnormal grains emerge and the mechanism(s) driving their persistent growth advantage.

MM 21.9 Wed 17:45 H22

Direct Laser Writing of metallic material utilizing the principle of sensitized triplet-triplet upconversion — •Kristin E. J. Kühl[1] and Georg von Freymann[1,2] — [1]University of Kaiserslautern-Landau, 67663 Kaiserslautern — [2]Fraunhofer Institute for Industrial Mathematics ITWM, 67663 Kaiserslautern

Direct Laser Writing (DLW) is a versatile technique for fabrication of microstructures, which is constantly evolving. Conventional DLW uses two photon absorption to form polymers from monomers via a photochemical reaction. Current research is leaning towards new materials, such as different kinds of metal which satisfy different demands on the physical properties of structures like electric conductivity or ferromagnetism, as well as the application of different photochemical reactions to provide more opportunities in the implementation of the printing process.

In this talk a novel approach to Direct Laser Writing of metallic materials is presented. For this purpose, photochemical compounds and principles were investigated via different methods and applied in a home built setup for Direct Laser Writing. A sensitized triplet-triplet annihilation upconversion process (sTTA-UC) is used to generate the energy required for the photochemical reduction of nickel. Since efficient sTTA-UC is usually limited to deoxygenated materials, a solvent is used that has the property of generating a local deoxygenated area upon excitation by a sensitizer. These three processes are combined to enable Direct Laser Writing of 2D nickel structures.

MM 21.10 Wed 18:00 H22

Friction coefficient and work function investigation of transition-metal dichalcogenide — •Malik Al naabi, Shuyu Huang, Antoine Hinaut, Ernst Meyer, and Thilo Glatzel — University of Basel, Basel, Switzerland

Despite extensive research on the tribological properties of MoS2,the frictional characteristics and electronic properties of other members of the transition-metal dichalcogenide (TMD) family have remained relatively unexplored. To understand the effect of the chalcogen on the tribological behavior of these materials and gain broader general insights into the factors controlling friction at the nanoscale, we compared the friction force behavior for a nanoscale single asperity sliding on MoS2, MoSe2, WS2, and WSe2, in bulk using friction force microscopy (FFM). Additionally, we used Kelvin probe force microscopy (KPFM) to investigate the work function. All the materials were cleaved in the nitrogen glovebox.

MM 21.11 Wed 18:15 H22

Nano-scale precipitations in NiTi-based alloys after laser powder bed fusion: FIB/STEM and APT analyses — •Farzad Khodabakhshi[1], Raphael Freundl[2], Eric A. Jägle[2], and Gerhard Wilde[1] — [1]University of Muenster — [2]Universität der Bundeswehr München

Phase formation and nano-scale precipitation during laser powder bed fusion (LPBF) of a NiTi/Nb powder mixture were characterized throughout the matrix of NiTi using advanced microscopy techniques. The study employed focused ion beam (FIB) preparation combined with scanning transmission electron microscopy (STEM) and atom probe tomography (APT). Different nano-scale phases formed through in situ alloying and their interfacial coherence with the NiTi-based alloy were examined using atomic-scale high-resolution microscopy. Subsequent nano-scale elemental mapping and chemical analysis were performed by APT. The results indicated significant changes in the contributions of in situ formed phases when altering the fraction of niobium. Low fractions of Nb can modify the intrinsic structure of NiTi precipitates. Changing the grain boundary energy helps shift these precipitates toward the interiors of grains rather than remaining at the boundaries. Conversely, increasing the niobium fraction towards the eutectic composition results in the formation of a new structure comprised of precipitates with a specific ternary composition within the NiTi alloy matrix due to LPBF deposition.

MM 22: Materials for the Storage and Conversion of Energy

Time: Wednesday 15:45–16:45 Location: H23

MM 22.1 Wed 15:45 H23

Understanding Stability of Ni-rich NMC cathodes using beyond DFT many-body calculatations

— •Hrishit Banerjee[1,2,3,4], Clare Grey[2,4], and Andrew Morris[3,4] — [1]University of Dundee — [2]University of Cambridge — [3]University of Birmingham — [4]The Faraday Institution

High energy density Ni-rich $\mathrm{LiNi}_a\mathrm{Mn}_b\mathrm{Co}_c\mathrm{O}_2$ (NMC) cathodes undergo degradation in the form of O loss from the surface of NMC particles. O loss increases with Ni content and higher voltages. Our first-principles study examines the redox behavior of transition metals and O in NMC cathodes as a function of (de)lithiation. Despite Ni, Mn, and Co K-edges calculated using GW Approximation showing an excellent match with experimentally obtained XANES, we demonstrate that the ionic model of ascribing shifts in the XANES to changes in metal oxidation states is inappropriate. In these cases, which are characterised by strong covalency between the strongly correlated transition metal and oxygen, Dynamical Mean-Field Theory calculations are essential to calculate charges and hence assign oxidation states accurately. Due to a charge transfer from O p to Ni d, a ligand hole forms on O in Ni-rich regions. The individual Ni charge remains fairly constant throughout the charging/discharging process. In contrast, O has dual redox behavior, showing greater involvement in redox in Ni-rich regions while showing negligible redox involvement in Ni-poor regions. The dual behaviour of O in terms of participation in the redox process explains the overall higher relative stability of lower Ni content NMCs compared to Ni-rich NMCs or LiNiO_2 in terms of O loss.

MM 22.2 Wed 16:00 H23

Splitting Water Without Falling Apart: Accelerating the Understanding of NiFeV LDH via Design of Experiments and Machine Learning

— •Juan Manuel Lombardi, Charles Pare, Karsten Reuter, and Christoph Scheurer — Fritz-Haber-Institut der MPG, Berlin

The development of sustainable energy technologies requires efficient, affordable, and durable electrocatalysts. Ni-based layered double hydroxides (LDHs) doped with Fe and V are promising candidates for the oxygen evolution reaction in anion exchange membrane water electrolyzers (AEMWE) due to their tunable structure and exceptional redox properties. However, the mechanisms by which dopants influence catalytic and structural properties are not fully understood, mainly due to the challenges posed by their humongous configurational space. In this study, we efficiently explore the thermally accessible configurations within the complex configurational space of γ-phase Ni LDHs doped with Fe and V. To maximize information gain, we sample the composition space using Design of Experiments (DoE), leverage machine learning interatomic potentials (MLIPs) to sample these configurations, and refine the results with Density Functional Theory (DFT) calculations for first-principles quality predictions. By combining these tools, we develop an optimal protocol to elucidate how the dopants influence material properties. This integrated methodology reveals pathways for optimizing NiFeV LDH compositions, enhancing energy conversion efficiencies while ensuring long-term stability.

MM 22.3 Wed 16:15 H23

Benchmarking exchange-correlation functionals for accurate computational predictions of metal organic frameworks

— •Julia Santana Andreo, Joshua Edzards, Holger-Dietrich Sassnick, and Caterina Cocchi — Carl von Ossietzky Universität Oldenburg, Institute of Physics

Metal-organic frameworks (MOFs) have attracted significant attention due to their structural and chemical flexibility which makes them relevant for a wide range of technological applications, from gas storage to photocatalysis. The substitution of metal nodes and the functionalization of organic linkers can significantly expand the range of available MOFs, enabling the design of tailored properties for specific applications. While atomistic ab initio simulations can significantly contribute to explore this vast configurational space, it is mandatory to assess whether and how common approximations of density-functional-theory calculations affect the description of the structural, electronic, and vibrational properties of computationally predicted compounds. With the example of MOF-5 and its recently predicted functionalized variants [1] , we find that R2SCAN offers the optimal trade-off between accuracy and computational costs to describe electronic and vibrational properties in these materials.

[1] J. Edzards, H.-D. Saßnick, J. S. Andreo and C. Cocchi, J. Chem. Phys. 160, 184706 (2024)

MM 22.4 Wed 16:30 H23

Assessing the Bulk Stability of Oxygen Evolution Reaction Catalysts using Crystal Field Theory and Orbital Analysis

— •Katarina Kretschmer[1], Michael Eikerling[1,2], and Tobias Binninger[1] — [1]Theory and Computation of Energy Materials (IET-3), Institute of Energy Technologies, Forschungszentrum Jülich GmbH, 52425 Jülich, Germany — [2]Chair of Theory and Computation of Energy Materials, Faculty of Georesources and Materials Engineering, RWTH Aachen University, 52072 Aachen, Germany

Proton exchange membrane water electrolysis (PEMWE) is an effective method for producing green, i.e. carbon-neutral hydrogen. At the PEMWE anode catalyst, water molecules are split to form oxygen molecules in the so-called oxygen evolution reaction (OER). Iridium oxide (IrO2) and ruthenium oxide (RuO2) are recognized as highly effective catalysts for the OER.

In this talk, I will discuss the electronic properties governing the bulk stability if IrO2 and RuO2. Utilizing density functional theory (DFT) calculations, the stability of both oxide materials is assessed from the perspective of crystal field theory and bond orbital analysis. The orbital overlap between the metal (iridium or ruthenium) and oxygen atoms in the lattice and the population of the emerging bonding or antibonding orbitals is analyzed, which can either contribute to or counteract the stability of the IrO2 and RuO2 lattices. This analysis will lead to the definition of electronic descriptors for predicting the bulk stability of transition metal oxide catalysts.

MM 23: Phase Transformations

Time: Wednesday 17:15–18:30 Location: H23

MM 23.1 Wed 17:15 H23

study on solid/liquid interfacial energy of Al-Cu alloys and its anisotropy under a static magnetic fields — •Chenglin Huang[1], Peter Galenko[2], Rainer Backofen[3], Ken Elder[4], Sansan Shuai[1], Jiang Wang[1], and Zhongming Ren[1] — [1]State Key Laboratory of Advanced Special Steel, School of Materials Science and Engineering, Shanghai University, 200444, P. R. C — [2]Department of Physics and Astronomy, Friedrich Schiller University of Jena, 07743, Germany — [3]Institute of Scientific Computing, Technische Universität Dresden, 01062 , Germany — [4]Department of Physics, Oakland University, Rochester, MI, 48309-4487, USA

In recent decades, external magnetic fields have been widely used in materials processing to control microstructure and optimize properties. Key phenomena include magnetic levitation, crystallographic orientation changes, magnetically induced phase transitions, and TEMHD. External magnetic fields also impact thermophysical properties such as phase transition temperatures, resistivity, viscosity, diffusion, and surface tension. These effects are closely linked to interface changes, where properties differ from the bulk. Despite their importance, quantitative studies on solid/liquid interfaces under magnetic fields remain limited. Accurately measuring interfacial energy and anisotropy, and exploring atomic-scale behavior under magnetic fields, are key challenges. This research systematically investigates the effects of external magnetic fields on interfacial energy and its anisotropy in Al-Cu alloys, offering theoretical and practical insights for controlling solidification under such fields.

MM 23.2 Wed 17:30 H23

From electronic structure to thermodynamic phase diagrams with automated workflows — •Sarath Menon[1], Marvin Poul[1], Tilmann Hickel[2], Ralf Drautz[3], and Jörg Neugebauer[1] — [1]Max Planck Institute for Sustainable Materials — [2]Bundesanstalt für Materialforschung und -prüfung — [3]Ruhr University Bochum

Phase diagrams are useful for understanding coexistence lines, phase stability, and phase transitions under varying thermodynamic conditions. Calculating phase diagrams involves determining the Helmholtz and Gibbs free energies of different phases and their dependence on thermodynamic state variables - a task that is both intricate and computationally demanding.

In this work, we introduce automated workflows for the calculation of Helmholtz and Gibbs free energies, incorporating configurational entropy, and provide accompanying computational tools. A key component of our approach is the alchemical transformation method, where atomic species are systematically altered along a thermodynamic path to evaluate free energy changes with composition.

We demonstrate the effectiveness of this methodology using an Atomic Cluster Expansion (ACE) machine-learning interatomic potential, parametrized using the ASSYST method, to generate unbiased *ab initio* structure datasets, and compute the phase diagram of the Au-Cu system. Our workflows are independent of the interatomic potential and the material system, making them readily transferable and paving the way for making the computation of thermodynamic phase diagrams a routine task in the field of atomistic simulations.

MM 23.3 Wed 17:45 H23

Phase formation at an interface between Ni and Sn layers during a soldering process — •Sandra Gaertner, Sergiy V. Divinski, Harald Rösner, and Gehard Wilde — Institute of Materials Physics, University of Münster, Münster, Germany

Soldering is a method for creating permanent bonds between metal parts, often resulting in the formation of intermetallic compounds. The transition to lead-free solder, driven by environmental regulations, has increased the interest in Sn-based solder alloys. However, the soldering process for interconnects involves complex processes related to material transport, phase stability, phase formation, and kinetic aspects of phase transformation. In this study, we investigated the interdiffusion and diffusion-controlled phase formation in a SnSb-solder alloy between a Ni-based layer with a small amount of Si and a Cu substrate, employing SEM and TEM. Analysis of the untreated states revealed a lamellar-type structure of the Ni-based layer, characterized by a uniform distribution of elements, while the solder alloy exhibited a β-Sn matrix and a SbSn phase. Following the soldering process, we observed the formation of various intermetallic compounds like CuSnNi and SnCu, encased within the β-Sn matrix. The SbSn phase remained as small inclusions. Moreover, the Ni-based layer initially shrank, resulting in a residual thin film that displayed an increased Si content compared to its untreated counterpart. This study highlights the intricate mechanisms involved in Cu transport from the substrate through the solder material. Alongside Sn, Cu drives the transformation of the Ni-based layer, ultimately leading to its complete consumption.

MM 23.4 Wed 18:00 H23

Temperature-modulated dilatometry as a tool for studying precipitation kinetics in alloys — •Marcel Simhofer[1], Philipp Brunner[1], Jiehua Li[2], Wolfgang Sprengel[1], and Roland Würschum[1] — [1]Inst. of Mater. Phys., NAWI Graz, Graz Univ. of Technol., Graz 8010, Austria — [2]Inst. of Casting Res., Montanuniv. Leoben, Leoben 8700, Austria

Temperature-modulated dilatometry is implemented as a tool for studying phase equilibration processes in alloys. As a case example, the phase equilibration between the saturated solid solution Al(Mg) and intermetallic Al_3Mg_2 in the Al(Mg) binary alloy is studied. The varying solubility of Mg in Al upon temperature modulation causes a modulation of the relative fractions of the two phases, which can be in-situ monitored by dilatometry owing to their different atomic volumes. The phase shift between the length change caused by phase equilibration and the applied sinusoidal temperature variation yields access to equilibration kinetics. The observed variation of the phase shift with the modulation frequency is quantitatively analyzed in the framework of a simple kinetic model, revealing that the equilibration process is controlled by the diffusion of Mg in Al.

M. Simhofer et al., J.Alloys&Comp. 1010 (2025) 176984

MM 23.5 Wed 18:15 H23

Formation mechanism of bicontinuous structure during peritectic melting of TiAg — •Zhongyang Li[1], Lukas Lührs[1], Tobias Krekeler[2], and Jörg Weissmüller[1,3] — [1]Institute of Materials Physics and Technology, Hamburg University of Technology, Hamburg, Germany — [2]Electron Microscopy Unit, Hamburg University of Technology, Hamburg, Germany — [3]Institute of Hydrogen Technology, Helmholtz-Zentrum Hereon, Geesthacht, Germany

Reverse peritectic reactions, and specifically the peritectic melting of TiAg, have been proposed as dealloying-like processes that produce quite similar microstructures but avoid the restrictions on sample size inherent in liquid-metal dealloying (LMD). Here, studies of the microstructure evolution during peritectic melting of TiAg suggest a formation mechanism that is not LMD-like but rather relies on liquid film migration. The process starts with wetting of the TiAg grain boundaries by the alloy melt. Successively, both Ti and Ag continue to dissolve from one side of, while β-Ti deposits on the other side and the liquid film sweeps the pristine TiAg crystal. TiAg-Ti interfaces with well-defined orientation relationship and with concentration gradients support this picture, as does the phase morphology in partly decomposed samples. The process generates a bicontinuous structure with a solid Ti skeleton, interpenetrated by the Ag-rich melt, which is conserved even after coarsening. This study clarifies the mechanism of peritectic melting in TiAg, and it may provide a basis for identifying other alloy systems suitable for producing bicontinuous microstructures by that process.

MM 24: Members' Assembly

Welcome to this general meeting of the DPG-SKM division MM! All of you, presenters of MM talks or posters and other interested participants of this conference, are cordially invited to this meeting. We will come together in a relaxed atmosphere, supported by drinks and pretzels (at least) for personal exchange. The poster prizes will be awarded during the Members Assembly. The current conference will be discussed and your feedback is very welcome. We will ask for your suggestions for future topical sessions in MM and symposia as well as for invited speakers. Take this opportunity to share your ideas regarding our MM program for our next DPG spring meeting.

Time: Wednesday 18:45–20:45 Location: H10

All members of the Metal and Material Physics Division are invited to participate.

MM 25: Invited Talk: D. Rodney

Time: Thursday 9:30–10:00 Location: H10

Invited Talk MM 25.1 Thu 9:30 H10

Transformation-induced plasticity in zirconia ceramics: neural network simulations and in-situ experiments — •David Rodney — Institut Lumière Matière, Université de Lyon, France

Brittleness limits the structural use of ceramics, but zirconia stands out due to transformation-induced plasticity (TRIP) between tetragonal and monoclinic phases. This stress-driven transformation enables up to 7% plastic deformation in single-crystalline ceria-doped zirconia, offering potential for high ductility. However, understanding the TRIP effect remains incomplete.

To address this, we combined in situ Laue micro-diffraction experiments at synchrotron facilities with atomistic simulations. Existing interatomic potentials fail to capture zirconia's complex polymorphism. We thus developed neural network interatomic potentials (NNIP) using DeepMD-kit for pure and ceria-doped zirconia. These NNIPs align well with ab initio data on thermodynamic, mechanical, and dynamical properties, accurately modeling phase stability, elastic properties, and energy barriers.

Using the NNIPs, we simulated the uniaxial compression of tetragonal ceramics, exploring stress-strain behavior, phase transformations, and deformation mechanisms across various compression directions. Simulations are confronted with the in situ experiments and the phenomenological theory of martensitic transformation. Key factors, including size, temperature, strain rate, and pre-existing defects, are critically analyzed, providing a comprehensive understanding of stress-induced phase transformations in zirconia ceramics.

MM 26: Topical Session: Thermophysical Properties of Bulk Metallic Glasses and Bulk Metallic Glass-forming Liquids

Time: Thursday 10:15–11:45 Location: H10

MM 26.1 Thu 10:15 H10

Influence of sulfur on the amorphous structure, high temperature viscosity and solidification of Zr-based bulk metallic glass formers — •Bastian Adam, Oliver Kruse, Lucas Mathias Ruschel, Maximillian Frey, Nico Neuber, and Ralf Busch — Chair of Metallic materials (LMW), Saarbrücken, Germany

The usage of the element sulfur in Bulk Metallic Glass (BMG) synthesis was recently introduced by Kuball et al. and lead to increased research interest into these new family of BMG [1]. Here we report on the influence of sulfur on the A2B type intermetallic composition (Zr50Ti16.6Ni18.3Cu15) that was characterized by container-less electromagnetic melting under microgravity within the 43rd & 44th TEMPUS parabolic flight campaigns by the German aerospace center (DLR). The investigation is accompanied by structural investigations of the amorphous solid and liquid that were conducted with the help of an electrostatic levitation device to observe the structure and solidification in an in-situ wide-angle scattering diffraction experiment at the German electron synchrotron (DESY) in Hamburg.

[1]A. Kuball, O. Gross, B. Bochtler, and R. Busch, Sulfur-bearing metallic glasses: A new family of bulk glass-forming alloys, Scr. Mater., 2018.

MM 26.2 Thu 10:30 H10

Structure and dynamics of Ni-Nb alloy melts upon sulfur addition — Nicolai Grund[1], Dirk Holland-Moritz[1], Saba Khademorezaian[2], Lucas P. Kreuzer[1,3], Nico Neuber[4], Lucas M. Ruschel[4], Hendrik Voigt[2], Johanna Wilden[1], •Fan Yang[1], Sergiy Divinski[2], Ralf Busch[4], Andreas Meyer[1], and Gerhard Wilde[2] — [1]Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt (DLR), Köln, Germany — [2]Institute of Materials Physics, University of Münster, Münster, Germany — [3]Heinz Maier-Leibnitz-Zentrum, Technische Universität München, Garching, Germany — [4]Chair of Metallic Materials, Saarland University, Saarbrücken, Germany

We investigated the change in the structure and dynamics of a Ni-Nb bulk metallic glass upon sulfur addition on microscopic and macroscopic scales. With the sulfur concentration of 3 at.%, where the composition $Ni_{58}Nb_{39}S_3$ exhibits the best glass forming ability in the investigated sulfur concentration range, both the equilibrium and undercooled melt dynamics remain almost unchanged. Only in the glassy state sulfur seems to result in less decoupled mass transport to the viscosity of the undercooled liquid, where the Ag tracer diffusion coefficient is slower in the ternary alloy. With the structural disorder introduced by alloying sulfur, the improved glass forming ability is attributed to geometrical frustration, where crystal nucleation requires a depletion of sulfur and hence long range diffusion, as long as no primary sulfur-containing crystalline phase is involved.

MM 26.3 Thu 10:45 H10

Probing Medium-Range Order in Metallic Glasses with 4D-STEM — •Birte Riechers[1] and Robert Maass[1,2,3] — [1]Federal Institute of Materials Research and Testing (BAM), Germany — [2]University of Illinois at Urbana-Champaign, USA — [3]Technical University of Munich, Germany

Medium-range order (MRO) in metallic glasses (MGs) plays a crucial role for their applicability, as it significantly affects their mechanical properties. Important details of the MRO were revealed by micro-second long atomistic simulations, that have shed light on the temperature- and time-dependent evolution of MRO, especially in connection to the emergence of a network of specific structural motifs (JALCOM 821, 153209, 2020; Acta Mater. 267, 119730, 2024).

While these insights help to understand the effect of MRO evolution, the experimental validation remains challenging. To test these findings, we employ 4-dimensional scanning transmission electron microscopy (4D-STEM) (Ultramicroscopy 232, 113405, 2022) to analyze both the first and second diffraction shells of MGs. By examining the diffraction symmetries at these length scales, we aim to uncover the dominant structural features associated with MRO.

MM 26.4 Thu 11:00 H10

Structural evolution during annealing in a Zr-Cu-Al bulk metallic glass by X-ray absorption spectroscopy — •Andrea Fantin, Reza Rashidi, Birte Riechers, and Robert Maass — Bundesanstalt fuer Materialforschung und -pruefung, Unter den Eichen 87, 12205 Berlin, Germany

Understanding structural evolution in the time-temperature-transformation diagrams of bulk metallic glasses (BMGs) is crucial to tackle common challenges in glass science such as embrittlement and mechanical failure. Preliminary extended X-ray absorption spectroscopy fine structure (EXAFS) measurements carried out at the Zr and Cu K-edges on a typical Zr-Cu-Al system allowed following the evolution of element-specific bond lengths, static and dynamic disorder, and nearest-neighbor numbers as a function of temperature and time. Data on the as-cast BMG, on further annealed BMG at two different temperatures (0.9Tg and 1.02Tg) and at different holding times was collected (ex-situ) at the BM-08 beamline, ESRF, finally showing two different behaviors depending on the temperature used, which will be described in terms of EXAFS fitting parameters during the presentation.

MM 26.5 Thu 11:15 H10

Thermodynamic, kinetic and structural study of Pt42.5CuxNi36.5-xP21 alloy variations — •Ziyu Ling[1], Maryam Rahimi Chegeni[1], Nico Neuber[1], Sergey Kasatikov[2], Amirhossein Ghavimi[1], Andrea Fantin[3], Isabella Gallino[4], and Ralf Busch[1] — [1]Lehrstuhl für Metallische Werkstoffe, Universität des Saarlandes — [2]Helmholtz-Zentrum Berlin für Materialien und Energie Elektrochemische Energiespeicherung — [3]Bundesanstalt für Materialforschung und -prüfung, Berlin — [4]Lehrstuhl für Metallische Werkstoffe,TU Berlin

The thermodynamic and kinetic properties of Pt42.5CuxNi36.5-xP21 glass-forming liquids are studied via differential scanning calorimetry and Flash DSC (Mettler Toledo). The kinetic fragilities of the alloys are determined from relaxation times measured in a broad heating rates range using a Tg shift method and the relaxation time of the deeply undercooled liquids determined via a step-response method. Furthermore, the specific capacity heat (Cp) as a function of temperature for the glassy, liquid and crystalline state of the chosen alloys are determined. The thermodynamic fragility is assessed from the 'Cp jump' at Tg and the driving force for crystallization is calculated using fitting parameters of thermodynamic functions derived from Cp data. Then the glass forming ability of the alloy liquids is evaluated based on their critical cooling rates and TTT-diagrams. The interfacial energy is obtained by JMAK fitting with TTT-diagrams. Moreover, the alloy ribbons were investigated by synchrotron X-ray scattering experiments at DESY for structural study and by XPS and NEXAFS at BESSY for energy state information of each elements.

MM 26.6 Thu 11:30 H10

Temperature dependence of cooperativ fluctuations in supercooled glass-forming metallic melts — •Jürgen Schawe[1], Min Kyung Kwak[2], Mihai Stoica[1], Eun Soo Park[2], and Jörg Löffler[1] — [1]ETH Zürich, Laboratory of Metal Physics and Technology, Zurich, Switzerland — [2]Seoul National University, Department of Materials Science and Engineering, Seoul, Republic of Korea

The behavior of a supercooled glass-forming metal alloy depends on the cooperative atomic fluctuations caused by the dynamic heterogeneities in the melt. These spatial and temporal heterogeneities form dynamic clusters, which are regions of cooperative rearrangement (CRR). The time and temperature dependence of the CRR characterizes the α-relaxation. In this study, the correlation length ξ, characteristic of the CRR, is derived for Pt57.4Cu14.7Ni5.3P22.6 and Pd43Cu27Ni10P20 bulk metallic glasses by fast differential scanning calorimetry in a temperature range between the glass transition temperature Tg and Tg + 50K. It appears that while the composition of the alloy influences the macroscopic α-relaxation and vitrification kinetics, typically defined by Tg, as well as the limiting temperature of the Vogel-Fulcher-Tammann-Hesse equation and the fragility index, it has no significant influence on the correlation length of the cooperative atomic motions. In agreement with many other materials, ξ at Tg is about 3 nm for both metallic glasses. The temperature dependence of ξ correlates with the apparent activation energy of the α-relaxation and is the reason for their non-Arrhenius behavior.

MM 27: Transport in Materials: Diffusion, Charge or Heat Conduction

Machine Learning, Quantum Theory

Time: Thursday 10:15–13:00 Location: H22

MM 27.1 Thu 10:15 H22

Modelling Heat Transport in Metal-Organic Frameworks with Machine Learned Potentials — •Martin Klotz[1], Florian Lindner[1], Sandro Wieser[2], and Egbert Zojer[1] — [1]Institute of Solid State Physics, Graz University of Technology, Austria — [2]Institute of Materials Chemistry, TU Wien, Austria

Many of the envisioned applications of porous metal-organic frameworks (MOFs), like gas storage or catalysis, involve exothermal processes. This requires the materials to efficiently dissipate heat. It is, thus, vital to gain a fundamental understanding of how structural and chemical modifications impact heat-transport in such systems. Here, we chose MOF-74/Zn as parent system for which we calculated the anisotropic thermal conductivity using approach to equilibrium molecular dynamics simulations. For these, we applied machine-learned force field potentials, as they surpass DFT simulations by orders of magnitudes in terms of speed and classically parametrized force field potentials in terms of accuracy. Subsequent to thoroughly benchmarking and testing the employed methodology, we studied structure-to-property relationships for MOF-74 derivatives, systematically varying the node metal and the linker structure.

MM 27.2 Thu 10:30 H22

Predicting 2D conventional superconductors — Thalis H. B. da Silva[1], Théo Cavignac[2], Tiago F. T. Cerqueira[1], •Hai-Chen Wang[2], and Miguel A. L. Marques[2] — [1]CFisUC, Department of Physics, University of Coimbra, Rua Larga, 3004-516 Coimbra, Portugal — [2]Universitätsstr. 150

We perform a large-scale search for two-dimensional (2D) superconductors by using electron-phonon calculations with density-functional perturbation theory combined with machine learning models. In total, we screened over 140k 2D compounds from the Alexandria database. Our high-throughput approach revealed a multitude of 2D superconductors with diverse chemistries and crystal structures. Moreover, we find that 2D materials generally exhibit stronger electron-phonon coupling than their 3D counterparts, although their average phonon frequencies are lower, leading to an overall lower transition temperature (T_c). Despite this, we discovered several out-of-distribution materials with relatively high T_c. In total, 105 2D systems were found with $T_c > 5$ K. Some interesting compounds, such as CuH_2, NbN, and V_2NS_2, demonstrate high T_c values and good thermodynamic stability, making them strong candidates for experimental synthesis and practical applications. Our findings highlight the critical role of computational databases and machine learning in accelerating the discovery of novel superconductors.

MM 27.3 Thu 10:45 H22

Modelling complex proton transport phenomena - Exploring the limits of fine-tuning and transferability of foundational machine-learned force fields — •Christian Dressler[1], Malte Grunert[2], Jonas Hänseroth[1], Max Grossmann[2], and Erich Runge[2] — [1]TU Ilmenau, Institute of Physics, Theoretical Solid State Physics — [2]TU Ilmenau, Institute of Physics, Group of Theoretical Physics 1

The solid acids CsH_2PO_4 and $Cs_7(H_4PO_4)(H_2PO_4)_8$ pose significant challenges for the simulation of proton transport phenomena. In this talk, we present the use of the recently developed machine-learned force field MACE to model proton dynamics on nanosecond timescales for these systems and compare its performance with long-term ab initio molecular dynamics (AIMD) simulations. The MACE-MP-0 foundation model shows remarkable performance for all observables derived from molecular dynamics simulations, but minor quantitative discrepancies remain compared to the AIMD reference data. However, we show that minimal fine-tuning - fitting to as little as 1 ps of AIMD data - leads to full quantitative agreement between the radial distribution and autocorrelation functions of MACE force field and AIMD simulations. Long-time AIMD simulations are unable to capture the correct qualitative trends in diffusion coefficients due to their inherent time scale limitations. In contrast, we demonstrate that accurate and convergent diffusion coefficients, consistent with experimental data, can only be reliably achieved through multi-nanosecond molecular dynamics simulations utilizing machine-learned force fields.

MM 27.4 Thu 11:00 H22

Understanding thermal transport in organic semiconductors using machine learned force fields — •Florian Unterkofler[1], Lukas Reicht[1], Lukas Legenstein[1], Sandro Wieser[2], Michele Simoncelli[3], and Egbert Zojer[1] — [1]Graz University of Technology, Austria — [2]TU Wien, Austria — [3]Columbia University, New York (USA)

Organic semiconductors (OSCs) are key materials for optoelectronic devices such as solar cells and organic light-emitting diodes (OLEDs). While the properties related to charge transport of OSCs are relatively well understood, we still lack an understanding of the fundamentals of the heat transport in those materials. To study the atomistic origins of heat transport, we developed a strategy for calculating the thermal conductivity of complex organic crystals employing non-equilibrium molecular dynamics (NEMD) simulations with highly accurate, system-specific, machine-learned Moment Tensor Potentials (MTPs). These MTPs are trained on ab initio data obtained from on-the-fly active-learning molecular dynamics simulations.[1]

We then simulated the thermal transport in pentacene with NEMD to analyze the heat conduction in real space at an atomistic level and to identify heat-transport bottlenecks. Alternatively, we also use the MTPs to accurately calculate thermal conductivities arising from the particle-like propagation and the wave-like tunneling of phonons in reciprocal space. Both approaches are consistent and agree with available experiments.

[1] npj Comput Mater 10, 18 (2024)

MM 27.5 Thu 11:15 H22

Influence of Defects and Layer Twisting on Phonon Dynamics in Bilayer Graphene and MoS$_2$ Using Machine Learned-Force Field Calculations — •Sabuhi Badalov[1,2] and Harald Oberhofer[1,2] — [1]Department of Physics, University of Bayreuth — [2]Bavarian Center for Battery Technology, Bayreuth, Germany

In crystalline materials, thermal, mechanical and even electronic properties are often described in terms phonon spectra and dynamics. These, can, to a large degree be influenced by even minute structural changes, such as through defects or by altering the relative alignment of a material's layers. By means of a state-of-the-art machine learning-augmented force field approach, we carry out extensive phonon calculations to understand how the defect density and layer configurations influence the phonon spectra in bilayer graphene and MoS$_2$. Our results highlight an interplay of phononic phenomena with the materials' Moiré patterns with major consequences on the transport properties of these materials. Moreover, we explore the possibility of phonon-mediated superconductivity through the electron-phonon coupling in topologically nontrivial phonon states. While this is still ongoing research, our results so far not only further the understanding of phonon dynamics in 2D materials, but also offer a solid foundation for future investigations into harnessing topological phonons for advanced electronic and thermal control technologies.

15 min. break

MM 27.6 Thu 11:45 H22

Thermoelectric quantum transport simulations via the time-linear nonequilibrium Green's function method — •Riku Tuovinen[1] and Yaroslav Pavlyukh[2] — [1]Department of Physics, University of Jyväskylä, Finland — [2]Institute of Theoretical Physics, Wroclaw University of Science and Technology, Poland

Thermoelectric transport focuses on understanding charge and heat flow in quantum systems. While measuring electron current is relatively straightforward, nanoscale heat flux remains challenging to quantify [1]. Heat and charge exhibit fundamental differences, as highlighted by electron transport analysis within the nonequilibrium Green's function theory [2]. In the time-linear formulation, based on the generalized Kadanoff-Baym ansatz (GKBA), open system dynamics are described using an embedding correlator, enabling the calculation of time-dependent currents via the Meir-Wingreen formula [3]. However, calculating heat currents presents challenges, particularly within the wide-band limit approximation (WBLA), which can result in divergent energy integrals. Besides the mathematical issues, the WBLA's reliability depends on the physical properties of the leads. To address these limitations, we present thermoelectric quantum transport simulations using the time-linear GKBA method without relying on the WBLA [4].

[1] J. P. Pekola and B. Karimi, Rev. Mod. Phys. 93, 041001 (2021).
[2] M. Ridley et al., J. Phys. A: Math. Theor. 55, 273001 (2022).
[3] R. Tuovinen et al., Phys. Rev. Lett. 130, 246301 (2023).
[4] R. Tuovinen and Y. Pavlyukh, in preparation (2024).

MM 27.7 Thu 12:00 H22

Sublinear in temperature transport in kagome metals: interplay of Dirac cones and Van Hove singularities — •Nikolai Peshcherenko[1], Ning Mao[1], Claudia Felser[1], and Yang Zhang[2,3] — [1]Max Planck Institute for Chemical Physics of Solids, 01187, Dresden, Germany — [2]Department of Physics and Astronomy, University of Tennessee, Knoxville, TN 37996, USA — [3]Min H. Kao Department of Electrical Engineering and Computer Science, University of Tennessee, Knoxville, Tennessee 37996, USA

Kagome metals are known to host Dirac fermions and saddle point Van Hove singularities near Fermi level. With the minimal two-pocket model (Dirac cone + Van Hove singularity), we propose a semiclassical theory to explain the experimentally observed sublinear resistivity in Ni$_3$In and other Kagome metals. We derive the full semiclassical description of kinetic phenomena using Boltzmann equation, and demonstrate that internode electron-electron interaction leads to sublinear in T scaling for both electrical and thermal transport at low temperatures. At higher temperatures above the Dirac node chemical potential, thermal and electric currents dissipate through distinct scattering channels, making a ground for Wiedemann-Franz law violation.

MM 27.8 Thu 12:15 H22

Phonon induced heat transfer between gold nanogap electrodes — •Yuki Hanamura, Kazuma Kishimoto, Mizuki Tada, Ryo Yamada, and Hirokazu Tada — Graduate School of Engineering Science, Osaka University, Japan

Recent studies have observed anomalous increases in thermal conductance in nanogaps narrower than a few nanometers [1]. Theoretical models attribute this phenomenon to electron tunneling effects and propagation of lattice vibrations due to mechanical interactions between the electrodes, i.e., phonon transport [2]. Experimental difficulties in the nanoscale have prevented us from sufficiently understanding the heat transfer mechanisms.

We have developed a device to measure both thermal and electrical conductance across nanogap electrodes. The device comprises a suspended structure with Micro Electro Mechanical System (MEMS) based actuators to tune the gap distance. We observed increased thermal conductances in sufficiently separated nanogaps, even in the absence of electron tunneling, suggesting phonon transport as the dominant mechanism [3]. We will show the effects of electrode gap distance and temperature on heat transfer across the nanogap.

[1] M. Pascale et al., Appl. Phys. Lett. 122, 100501 (2023).
[2] T. Tokunaga et al., Phys. Rev. B 104, 125404 (2021).
[3] Y. Hanamura et al., Nanoscale, in press.

MM 27.9 Thu 12:30 H22

Hydrodynamics of Lorentz symmetric systems: a quantum Monte Carlo study — •Adrien Reingruber[1], Kitinan Pongsangangan[2], Fakher Assaad[1], and Maksim Ulybyshev[1] — [1]Universität Würzburg, Würzburg, Germany — [2]Mahidol University, Bangkok, Thailand

We present a study on the hydrodynamic behavior of charge current in a Lorentz symmetric sys- tem: graphene at charge-neutrality. The momentum flow is completely decoupled from the charge current in this regime, since the electrons and holes propagate in opposite directions with exactly equal distribution functions. Instead of Navier-Stokes equations for the velocity field, we derive sim- ilar equations directly for the charge current. This eliminates the need for any coupling between the velocity field and charge current to explain the experimentally observed hydrodynamic flow profiles in graphene at half-filling. In this framework, the current diffusion coefficient replaces viscosity. To support this, we performed an extensive quantum Monte Carlo study, directly simulating samples with disordered edges using the underlying microscopic interacting quantum Hamiltonian. For the first time, we observe hydrodynamic behavior of the charge current in such simulations, extract- ing current profiles and a current diffusion coefficient whose temperature dependence qualitatively agrees with predictions from Boltzmann transport theory.

MM 27.10 Thu 12:45 H22

Transport coefficients of Weyl semimetals: the contribution of plasmons — •Kitinan Pongsangangan — Mahidol University, Bangkok, Thailand

This work investigates the contribution of plasmon, a collective mode arising from the dynamical screening of the long-range coulomb interaction, to thermo-electric responses as well as shear viscosity of Weyl semimetals using Boltzmann-equation approach. We find that plasmons make a noticeable contribution to the thermal conductivity and shear viscosity in an appropriate temperature window. We propose that this effect could be potentially observed in, for example, TaAs and NbAs.

MM 28: Mechanical properties

Strengthening Mechanisms

Time: Thursday 10:15–11:30 Location: H23

MM 28.1 Thu 10:15 H23

Parameterising edge dislocation trajectories in Ni-based superalloys with uncertainty quantification — •Geraldine Anis, Thomas Hudson, and Peter Brommer — University of Warwick, Coventry, United Kingdom

The extraordinary strength exhibited by Ni-based superalloys at high temperatures is attributed to the presence of nanoscale precipitates in their microstructure, which hinder dislocation motion. In our work, we study edge dislocation-precipitate interactions using Molecular Dynamics (MD) simulations with classical effective potentials. The motion of a pair of edge dislocations moving under shear between pure Face-Centred Cubic (FCC) Ni into Ni3Al with an L12 structure is simulated using MD, where Ni is used to represent an idealised γ solid solution phase and Ni3Al for the γ' precipitate phase. The obtained trajectories are parameterised and Differential Evolution Monte Carlo (DE-MC) is used to determine parameter distributions. These distributions are then used to quantify the uncertainty in the model outputs, namely the dislocations' positions and velocities. The present approach yields physically meaningful parameters and accordingly, offers a means of extracting quantitative information from the atomistic scale that can be used to inform larger length scale simulations of dislocations. Using DE-MC as a sampling approach also means that parameter uncertainties can be propagated through a hierarchy of multiscale models. We illustrate how such uncertainty propagation can be achieved by considering a dislocation mobility law with quantified uncertainties.

MM 28.2 Thu 10:30 H23

Atomistic Modelling of Solid Solution Strengthening in the Mg-Al-Ca System — •Erik Bitzek and Marvin Poul — MPI SusMat, Düsseldorf, Germany

Solid solution strengthening is one of the most important strengthening mechanisms for engineering alloys. It is caused by solutes impeding the glide of dislocations and is therefore best studied using atomistic simulations. While the interaction strength of individual solute atoms with dislocations in Mg has been well-studied with density functional density (DFT) calculations, the combined impact of multiple solute species on dislocation glide has not been extensively investigated. Furthermore, the prediction of the critical resolved shear stress requires additionally a statistical treatment and a continuum elastic model for the dislocation line.

Here we present atomistic simulations of basal dislocations gliding in Mg with different concentrations of Al, Ca, and mixtures of Al and Ca. These large-scale simulations were enabled by a newly-developed machine learning interatomic potential that allows for near-DFT accuracy. Using MD/MC simulations of different heat treatments, we show that Al-Ca clusters can form, which influence the solid solution strengthening by reducing the concentrations of individual solutes and through an antagonistic effect of Al and Ca on the stress field of these clusters.

MM 28.3 Thu 10:45 H23

Normal stress effect on the slip system of Mg alloys with long-period stacking ordered structures — •Naoki Uemura[1] and Ryosuke Matsumoto[2] — [1]Nagamori Institute of Actuators, Kyoto University of Advanced Science, Kyoto, Japan — [2]Department of Mechanical and Electrical Systems Engineering, Faculty of Engineering, Kyoto University of Advanced Science, Kyoto, Japan

Mg alloys with long-period stacking, which have a unique structure with synchronized concentration modulation and structural modulation are attracting attention for their high strength. Various studies are currently being conducted to understand their high mechanical properties and plastic deformation behaviors. We investigated the tensile and compressive dependence of the stacking fault energy (SFE) by using first-principles calculations for the Mg-Y-Zn system, which is a typical LPSO-Mg alloy. As with hcp-Mg, the change in SFE due to tensile and compressive loading was greater on the basal plane than on the prismatic plane. This work was supported by JST, CREST Grant Number JPMJCR2094, Japan.

MM 28.4 Thu 11:00 H23

Understanding crystal defects mechanisms with atomistic simulations and knowledge engineering — •Abril Azocar Guzman, Guojing Huang, and Stefan Sandfeld — Institute for Advanced Simulations, Materials Data Science and Informatics (IAS-9), Forschungszentrum Jülich GmbH, Aachen, Germany

Crystallographic defects play a key role for determining the physical properties of materials. Computational methods, such as density functional theory and molecular dynamics, have been widely used to investigate these defects and their mechanisms at the atomic scale. However, the application of these methods require increasingly complex workflows. To enable workflow and data reusability, as well as meaningful interpretation, it is crucial to ensure well-described (meta)data at each step of the workflow, from atomic structure to computed material properties. Our aim is to facilitate data-driven approaches in materials science by establishing semantic standards for representing material structures, including defects, simulation workflows, and calculated properties. Using this framework, datasets of crystal defects simulations can be generated in the form of a materials knowledge graph. We showcase the application for the study of hydrogen segregation at grain boundaries in iron and nickel, quantifying the influence of the local atomic environment on the energetics of the system. The resulting knowledge graph incorporates structure-property relationships and serves as a tool to understand defect mechanisms at the atomic scale. Additionally, it provides a robust data foundation for exploring the potential of emerging methods in the field of knowledge engineering.

MM 28.5 Thu 11:15 H23

Effect of Cold Work on the Microstructure and Properties of Hierarchical Nanoporous Metals — •Weiche Chang[1] and Shan Shi[2,1] — [1]Institute of Hydrogen Technology, Helmholtz-Zentrum Hereon, Geesthacht, Germany — [2]Research Group of Integrated Metallic Nanomaterials Systems, Hamburg University of Technology, Hamburg, Germany,

Nanoporous metals with bicontinuous porous network, high specific surface area, and low density have shown promising applications as light-weight structural materials and high-performance functional materials in actuators, sensors, and various energy devices. Recently, monolithic hierarchical nanoporous gold (HNPG) has been tailor-made via a two-step dealloying method and has shown improved mechanical properties and much lower density than non-hierarchical nanoporous gold. The effects of ligament size and structural hierarchy on the strength of HNPG have also been well studied via macro- or micro-compression approaches. In this work, we further explore the role of cold working treatments before and after second step dealloying on the mechanical properties of HNPG using micropillar compression tests. Furthermore, HNPG with a controllable degree of anisotropy and a much wider range of solid fractions are obtained.

MM 29: Liquid and Amorphous Materials

Time: Thursday 12:00–12:45 Location: H10

MM 29.1 Thu 12:00 H10

Molecular Feuds and Fragment Tales: Exploring Cyanobiphenyl Liquid Crystals with Cryo Atom Probe Tomography — •Kuan Meng, Kang'an Wang, Sebastian Eich, and Guido Schmitz — Stuttgart University,Institute for Materials Science, Heisenbergstr. 3, 70569, Stuttgart, Germany

Liquid crystals exhibit the fascinating duality of liquid-like fluidity and solid-like long-range order, requiring nanoscale characterization techniques with high spatial resolution and chemical sensitivity. Atom probe tomography (APT) uniquely meets these requirements, offering unprecedented insights into the behavior of anisotropic organic molecules. This talk bridges liquid crystal science and APT by exploring cyanobiphenyl systems (5CB, 8CB, and 8OCB).

We investigated the field evaporation behaviors of these molecules, observing remarkable stability under high electric fields. Molecular signals dominated (90% for 5CB and 8CB, 70% for 8OCB), with fragmentation patterns influenced by oxygen atoms. The fragments were classified as alkyl chains, single phenyl derivatives, cyanobiphenyl residues, and cyano-hydrogen substitution pairs. Spatially, both molecular and fragment signals correlate strongly with laser orientation: fragmentation decreases from illuminated to shadowed regions, reflecting cleavage behavior under thermal gradient-induced field variations. Additionally, APT revealed the uniform mixing of 5CB and 8CB across various ratios, as well as the lattice plane of the crystal structure of pure 8CB. In the crystalline regions, we will discuss how the molecules field evaporate at specific angles relative to their intrinsic orientations.

MM 29.2 Thu 12:15 H10

Peptide Analysis at Atomic Resolution with Atom Probe Tomography — •Sakshi Sinha and Guido Schmitz — Department of Materials Physics, Institute of Material Science, University of Stuttgart, Heisenbergstr. 3, 70569 Stuttgart

Atom Probe Tomography (APT) promise decisive advancements in nanoscale characterization of biomolecules, since it offers in principle single atom sensitivity in the study of organic molecular structures. In our experiments, we test the analysis of carnosine (β-alanylhistidine), in aqueous solution since water provides a natural biological environment. The investigated dipeptide is for example essential for brain and muscle function. By combining cryogenic sample preparation with advanced laser-pulsing techniques, APT enables three-dimensional mapping of carnosine's atomic composition and the distribution of various molecule fragments in the water matrix. Remarkably, the concentration of the solution controls the detected fragmentation behavior in the full range from single atoms to the full peptide molecule. So, the measurement conditions can be optimized to preferentially address the questions regarding the local stoichiometry or the different subunits of the molecule.

MM 29.3 Thu 12:30 H10

Fe self-diffusion in Fe-Al-Si melts - A combined ab initio molecular dynamics and experimental study — •Katharina Dammer[1], Fan Yang[1], Elke Sondermann[1], Florian Kargl[1], Andreas Meyer[1,2], and Noel Jakse[3] — [1]Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt (DLR), 51170 Köln, Germany — [2]Institut Laue-Langevin (ILL), 38042 Grenoble, France — [3]Université Grenoble Alpes, CNRS, Grenoble INP, SIMaP, 38000 Grenoble, France

Understanding the structural, dynamic and thermophysical properties of binary and ternary Al-Fe-Si alloys in the liquid and supercooled state before solidification is crucial to ensure the desired microstructure and therefore ideal product properties. With an increasing iron content in the alloy, the liquidus temperature increases and exceeds 1000°C for most ternary Al-Si-Fe alloys. At these high temperatures, experiments are more delicate to perform, making it challenging to obtain information on transport coefficients and (partial) structure factors.

We present a combined first principle-based molecular dynamics (AIMD) simulations and experimental study of Al-Fe melts. Measurements were performed using quasi elastic neutron scatting (QENS) to obtain the self-diffusion coefficients of Fe at different Al-Fe compositions as a function of temperature. We intend to achieve in the future an improved simulation scheme using machine learning that realistically covers a larger range of the phase diagram, which cannot be easily assessed with experiments.

MM 30: Functional Materials: Performance, Reliability and Degradation; and Complex Materials (joint session MM/KFM)

Time: Thursday 11:45–13:00 Location: H23

MM 30.1 Thu 11:45 H23

Untersuchungen des Bruchverhaltens im Bereich der Ultra-Langzeitfestigkeit von Federstählen — •Jörg Gollnick — THM, FB ME, Wiesenstr. 14, 35390 Gießen

In einer hochfrequenten resonanten Anwendung als Spiegel für Laserscanner werden Federstähle des Typs Ck101 im Grenzbereich belastet. Im Rahmen eines Forschungsvorhabens wurden die spezifischen Möglichkeiten untersucht, die Lebensdauer dieser Bauteile zu steigern. Bislang wurden nur unzureichende Lebensdauern erreicht.

Bemerkenswert war die Ausprägung des Versagensverhaltens, dass in Zusammenhang mit der Fertigungstechnologie einem Sprödbruch unter Mode III nach den bruchmechanischen Ansätzen gemäß Griffith entspricht. Aus der Erklärung der Schädigungen wurden weitere Möglichkeiten untersucht, die Lebensdauer nicht nur zu steigern sondern weiterhin die nach Paris-Erdogan zu erwartende Dauerfestigkeit genau zu bestimmen.

Mit hohen Frequenzen im Bereich bis zu 10000kHz werden Bauteile bis zu 10 Milliarden Schwingungen im Grenzbereich betrieben. Eine mehrstufige Auswertung nach dem Treppenstufenverfahren zeigt, dass eine Auswertung in diesem Segment nicht nur möglich ist, sondern als geeignete Strategie angesehen werden darf, die Erkenntnisse der Ultra-Langzeitfestigkeit diesbezüglich zu erweitern.

Weitergehende Versuche werden vorgestellt.

Falls gewünscht kann der Vortrag und Beitrag gerne auch auf englisch abgefasst werden.

MM 30.2 Thu 12:00 H23

Searching for ferroelectric porous metal organic frameworks using machine-learning and Monte-Carlo-simulations — •Thomas Bergler[1,2], Harald Oberhofer[1,2], and Dirk Volkmer[3] — [1]University of Bayreuth, Germany — [2]Bavarian Center for Battery Technologies — [3]University of Augsburg, Germany

Metal organic frameworks (MOFs) have so far found a number of successful applications, among them as storage for gasses and filter for gas mixtures. So far these mostly incorporated them as passive materials, but recent research points the way towards a more active role, possibly through the external manipulation of the materials' internal properties. One recent example for such a property is the susceptibility of the lattice parameters of a number of MOFs towards electric fields. Inspired by this, the aim of our project is to further investigate this behavior and potentially design ferroelectric MOFs. Using a hierarchy of Monte-Carlo-simulations aided by Machine-Learning (ML) we sample the design space MOFs augmented by rotatable polar groups. In succession, we first sample a huge space of rotors in a simplified point-dipole model. A selection of thus uncovered MOF geometries is then investigated with a specially parameterized atomistic model to confirm earlier predictions. Using this data, an ML model is trained to predict the dielectric properties of such polar rotor-augmented MOFs. The best candidates extracted with this procedure are finally evaluated with density functional theory. MOF geometries surviving this funnel-like approach can finally be checked experimentally for a variety of applications, ranging from data-storage to gas nano-funnelling.

MM 30.3 Thu 12:15 H23

Atomic Scale Insights into A-site Deficient Perovskite Catalysts:$La_{0.7}Fe_{0.7}Mn_{0.3}O_3$ — •Roham Talei Jeid — Institute for Material Physics, University of Stuttgart, Deutschland

This study investigates the atomic-scale properties of the A-site-deficient perovskite catalyst $La_{0.7}Fe_{0.7}Mn_{0.3}O_3$ (La07FM), emphasizing the role of iron oxide (FeO) in redox reactions. Advanced techniques, including scanning transmission electron microscopy (STEM), energy-dispersive X-ray spectroscopy (EDXS), and a custom Python-based strain mapping tool linked to chemical analysis reveal nanoscale La deficiencies and Fe enrichments at grain boundaries as key for catalytic activity. Post-catalysis studies identify Fe-rich, FeO-like nanoparticles at strained, defective grain boundaries, underscoring the impact of A-site deficiencies on performance in NOx denitrification (DeNOx). These findings highlight how A-site deficiencies and Fe-rich nanostructures enhance catalytic efficiency, offering broader insights into electrochemistry and heterogeneous catalysis.

MM 30.4 Thu 12:30 H23

Use of LiMn2O4 for switching applications in silicon waveguide circuits — •Vinit Agarwalla[1], Yug Joshi[2], and Guido Schmitz[1] — [1]Insitut für Materialwissenschaft, Universität Stuttgart, Heisenbergstr.3, 70569 Stuttgart — [2]Max-Planck-Institut für Nachhaltige Materialien, Max-Planck-Straße 1, 40237, Düsseldorf

Lithium ion intercalation and deintercalation play an important role in determining the storage performance of cathode materials for lithium ion batteries. However, intercalation of ions also regularly modifies electron structure and optical properties of the materials. This study explores the possibility of exploiting the optical properties of the cathode material LiMn2O4 (LMO) for optical switching applications in silicon waveguide circuits. For this, LMO is coated as a cladding around Si waveguides suitable for the 1550 nm wavelength of optical telecommunication. To stabilize the interface a thin intermediate Si oxide film is tested as an optical transparent reaction barrier. Our TEM images and the EDX mapping show that the Si does not react with LMO for oxide layer thickness as low as 10 nm. Previous work has explored the change in resonance wavelength of reflectance spectra with lithiation/delithiation in the visible region[1]. In extension, we have measured FTIR reflectance spectra in the near IR region. They show a fairly continuous spectrum between visible and IR region with reflectance going to 100 % and a gradual shift in resonance wavelength in the IR region with Li intercalation. The optical response on light transmission along the wave guides has been determined in dependence on the degree of lithiation. [1]. DOI:10.1002/adom.201701362

MM 30.5 Thu 12:45 H23

Chemical short-range order and local lattice distortions in High-Entropy Alloys: state of the art — •Andrea Fantin, Anna Maria Manzoni, Reza Darvishi Kamachali, and Robert Maass — Bundesanstalt fuer Materialforschung und -pruefung, Unter den Eichen 87, 12205 Berlin, Germany

Understanding the intricate atomic-scale structures within High-Entropy Alloys (HEAs) is crucial for tailoring their properties for diverse applications. This contribution tries to provide a brief overview of the state-of-the-art experimental techniques employed to probe local lattice distortions and chemical short-range order in HEAs, with specific focus on X-ray absorption spectroscopy and total scattering. The main problem to overcome in multi-component alloys is the intrinsic reduced scattering contrast between nearest neighbors in the periodic table, which limits the amount of information that can be extracted from the data. This statement remains valid when employing transmission electron microscopy, as well. Specific examples such as the Al-Co-Cr-Cu-Fe-Ni fcc system [Small Science 4(2), 2300225 (2024); Nature Communications 15(1), 7815 (2024)] and the MoNbTaW bcc system [Materials Research Letters 12(5), 346-354 (2024)] will be outlined. It comes clear that rather than specific techniques, it is only the combination of several experiments, supported by simulations and multi-technique simultaneous structural refinements, that can help in disentangling the different contributions to performances of each element within the alloy solid solution, with strength and weaknesses depending on the specific experimental measurements.

MM 31: Data-driven Materials Science: Big Data and Worksflows

Materials Properties and more

Time: Thursday 15:00–18:00 Location: H10

MM 31.1 Thu 15:00 H10

Thermodynamic stability of the materials in the Materials Cloud three-dimensional crystals database (MC3D) — •Timo Reents[1,2], Marnik Bercx[1], and Giovanni Pizzi[1,2] — [1]Laboratory for Materials Simulations (LMS) and National Centre for Computational Design and Discovery of Novel Materials (MARVEL), Paul Scherrer Institut (PSI), CH-5232 Villigen PSI, Switzerland — [2]École Polytechnique Fédérale de Lausanne (EPFL), Lausanne, Switzerland

High-throughput studies based on ab initio methods such as Density Functional Theory (DFT) enable the analysis of physical properties across a broad chemical space. Here, we present the Materials Cloud three-dimensional crystals database (MC3D), a DFT optimized and curated structural database of experimentally known inorganic crystals. All calculations are managed and driven by the AiiDA [1, 2] workflow engine, allowing to browse the full provenance graph and to share the results in the Materials Cloud [3]. We introduce the protocols behind MC3D, the new frontend, and we then focus on the thermodynamic stability. To improve the agreement between the theoretical and experimental thermodynamic stability, we apply empirical [4] and machine-learning [5] based corrections, and improve upon them, discussing the agreement with experimental data on stability.

[1] Huber, S.P. et al., Sci Data, 2020, 7, 300.
[2] Uhrin, M. et al., Comp. Mat. Sci., 2021, 187, 110086.
[3] Talirz, L. et al., Sci Data 7, 299 (2020).
[4] Stevanović, V. et al., Phys. Rev. B, 2012, 85, 115104.
[5] Gong, S. et al., JACS Au, 2022, 2, 1964-1977.

MM 31.2 Thu 15:15 H10

high-throughput computation and machine learning modeling of magnetic moments and Mössbauer spectroscopy for Fe-based intermetallics — •Bo Zhao, Xiankang Tang, and Hongbin Zhang — Institute of Materials Science, Technische Universität Darmstadt, Otto-Berndt-Str. 3, 64287 Darmstadt, Germany

Understanding the relationship between the local crystalline environment and magnetic properties is a fundamental challenge in condensed matter physics and materials science. This study explores this relationship in Fe-based intermetallic compounds, focusing on the magnetic moments and Mössbauer parameters of iron atoms, including the isomer shift, electric field gradient, and magnetic hyperfine field. High-throughput calculations and machine learning techniques are employed to predict magnetic properties based on local atomic structures, using smooth overlap of atomic positions (SOAP) as local descriptors. The results first reveal the sparsity of relevant materials in the Materials Project database. Leveraging high-throughput, system-specific data, the study demonstrates strong correlations between local atomic environments and magnetic properties, achieved through machine learning models. Furthermore, the limitations of symmetry-invariant descriptors in predicting tensor-like properties, such as the electric field gradient, are highlighted. By incorporating a graph-based equivariant autoencoder, the model achieves improved predictions by effectively capturing the symmetry of local environments.

MM 31.3 Thu 15:30 H10

Advanced Machine Learning of ^{17}O NMR in Non-Magnetic Oxides: High-Throughput Calculation, Prototype Compound Analysis, and Transfer Learning — •Zhiyuan Li, Bo Zhao, Hongbin Zhang, and Yixuan Zhang — Institute of Materials Science, TU Darmstadt, 64287 Darmstadt Germany

The study of ^{17}O NMR spectroscopy is crucial for understanding the local structure of oxides, where the naturally occurring NMR-active oxygen isotope, ^{17}O, provides unique insights into local environments due to its large chemical shift range and quadrupolar nature. In this work, we present a high-throughput workflow integrating AiiDa and CASTEP to calculate the NMR parameters of over 7100 compounds from the Materials Pro ject database, followed by utilizing machine learning models to predict ^{17}O NMR parameters. Furthermore, taking $BaTiO_3$ as an example, we identify prototypical ABO_3 crystal structures, construct $BaTiO_3$ analogs via substitution, perform ab initio molecular dynamics simulations to generate 3000 perturbated structures, and evaluate the NMR parameters. The results of our machine learning modeling with such additional dataset reveal that incorporating perturbated structures enhances the accuracy of the machine learning model. Moreover, by leveraging transfer learning, using previously trained model from our high-throughput dataset, the predictivity for the newly generated $BaTiO_3$ analogs can be further improved.

MM 31.4 Thu 15:45 H10

Advancing chemical shielding predictions in organic solids — •Matthias Kellner and Michele Ceriotti — École Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland

In this presentation, we showcase our recent advancements in machine learning for predicting chemical shieldings in organic solids. Leveraging symmetry-adapted machine learning models, our updated infrastructure facilitates the accurate prediction of chemical shielding anisotropy and enables structure optimization driven by chemical shielding gradients. We will highlight how integrating machine learning potentials with property prediction models provides unique insights into atomistic processes, offering a powerful framework for exploring the complex behavior of organic materials.

MM 31.5 Thu 16:00 H10

Active learning workflow for mixed-halide perovskite stability and electronic band-structure — •Tim Bechtel[1,2], Santiago Rigamonti[1], and Claudia Draxl[1,2] — [1]Humboldt-Universität zu Berlin, Germany — [2]Max Planck Institute for Solid-State Research, Stuttgart, Germany

Mixed-halide perovskites are promising materials for stable and efficient light harvesting and emission applications, and their composition can be tailored to match relevant regions of the light spectrum [1]. Theoretical predictions from first-principles calculations can provide insight into stability, ground-state properties, and electronic structure [2,3]. Comparison with experimental results for "real" materials is, however, challenging. For example, the consideration of chemical (dis)order requires huge supercells, which is computationally out of reach with state-of-the-art methodology. For the family of $CsPb(Cl_xBr_yI_{1-x-y})_3$ compounds, we bridge this gap with an active learning workflow. It is based on a fine-tuned machine learning interatomic potential [4] that interpolates between already seen compositions, and actively explores new composition ranges. This approach allows for data-efficient predictions of stability through finite-temperature phase diagrams and optical properties for a wide range of compositions.

[1] H. Näsström, PhD Thesis, https://doi.org/10.18452/24939
[2] F. Pan, *et al.*; https://doi.org/10.1021/acs.chemmater.4c00571
[3] J. Laakso, *et al.*; https://doi.org/10.1103/PhysRevMaterials.6.113801
[4] I. Batatia, *et al.*; https://doi.org/10.48550/arXiv.2401.00096

15 min. break

MM 31.6 Thu 16:30 H10

Towards Multi-Fidelity Machine Learning Using Robust Density Functional Tight Binding Models — •Mengnan Cui[1,2], Karsten Reuter[1], and Johannes T. Margraf[2] — [1]Fritz-Haber-Institut der MPG, Berlin, Germany — [2]University of Bayreuth, Physical Chemistry V: Theory and Machine Learning

Machine learning has revolutionized the atomistic simulation of molecules and materials, offering unparalleled computational speed with high accuracy. However, its performance depends heavily on the quality and quantity of training data, presenting challenges due to the scarcity of high-fidelity datasets (beyond semilocal DFT). This study investigates transfer learning (TL) across multiple fidelities for molecules and solids, examining the role of fidelity levels and configuration/chemical space overlap in pre-training and fine-tuning. This reveals negative transfer driven by noise from low-fidelity methods like DFTB, which can significantly impact fine-tuned models. Despite this, multi-fidelity approaches consistently outperform single-fidelity learning and, in some cases, even surpass TL based on foundation models by leveraging an optimal overlap of pre-training and fine-tuning chemical spaces.

MM 31.7 Thu 16:45 H10

Enhancing FAIR Data Management with Automated Visualization of Calculations — •N. Daelman[1], E. Boydas[1], B. Mohr[1], J.M. Pizarro[1], T. Bereau[2], C. Draxl[1], L.M. Ghiringhelli[3], M. Girard[4], D. Usvyat[5], R. Valenti[6], S. Botti[7], and J.F. Rudzinski[1] — [1]CSMB, HU Berlin — [2]ITP, Heidelberg Uni. — [3]Dept. of Mater. Sci. and Eng., FAU Erlangen — [4]Max Planck Inst. for Poly. Res., Mainz — [5]Inst. für Chem., HU Berlin — [6]Inst. für Theor. Phys., GU Frankfurt/M — [7]RC-FEMS, Ruhr Uni. Bochum

In contrast to data science packages, first-degree data post-processing tends to lock people into silos built around a particular simulation software. NOMAD [nomad-lab.eu][1] is an open-source and community-driven data infrastructure that breaks open these silos by extracting scientific data from over 60 code packages into a code-agnostic schema within a research data management (RDM) ecosystem [2]. This talk showcases NOMAD*s new visualization features at various levels of RDM. At the level of individual calculations, NOMAD provides now more detailed electronic structure visualizations and fast, dynamic rendering of heavy files. Automated visualization does not imply, however, a lack of customizability. NOMAD provides support for tailored figures and larger-scale specialization via an accessible plugin-based system. At the level of research projects, NOMAD allows for quick monitoring of the data coverage via a fully customizable dashboard.

[1] Scheidgen, M. *et al.*, JOSS **8**, 5388 (2023).
[2] Scheffler, M. *et al.*, Nature **604**, 635-642 (2022).

MM 31.8 Thu 17:00 H10

NOMAD CAMELS: An Open-Source Solution for Creating FAIR Data from Experiments — •Alexander Fuchs[1,2], Johannes Lehmeyer[1,2], Michael Krieger[1,2], and Heiko Weber[1,2] — [1]Lehrstuhl für Angewandte Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg — [2]FAIRmat Consortium

NOMAD CAMELS is a configurable open-source measurement software. It is suited to control experiments and records fully self-describing experimental data. It has its origins in the field of experimental physics where a wide variety of measurement instruments are used in frequently changing experimental setups and measurement protocols. CAMELS provides a graphical user interface (GUI) which allows the user to configure experiments without the need of programming skills or deep understanding of instrument communication. CAMELS translates user-defined measurement protocols into stand-alone executable Python code for full transparency of the actual measurement sequences. Metadata inflow from Electronic Lab Notebooks (ELNs) and data output into such is well supported for a seamless workflow. CAMELS is designed with a focus on full recording of data and metadata aligned with the NeXus ontology. When shared with others, data produced with CAMELS allow full understanding of the measurement and the resulting data in accordance with the FAIR principles.

MM 31.9 Thu 17:15 H10

Databases of Fermi surfaces and de Haas-van Alphen oscillation frequencies from first principles simulations — •Nataliya Paulish[1], Junfeng Qiao[2], and Giovanni Pizzi[1] — [1]PSI Center for Scientific Computing, Theory and Data, 5232 Villigen PSI, Switzerland — [2]Theory and Simulation of Materials (THEOS), and National Centre for Computational Design and Discovery of Novel Materials (MARVEL), École Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland

The Fermi surface (FS) of a metal separates occupied from unoccupied electronic states. Knowing its shape is crucial to understanding the electronic properties of the material. Accurate simulation of the FS requires a very dense sampling of the Brillouin zone, and thus direct density functional theory (DFT) calculations are limited by their computational cost. To overcome this difficulty, we use interpolation from a basis of spatially localized projectability disentangled Wannier functions (PDWFs) - a recently developed algorithm for automated Wannierization [1]. Using this algorithm, FSs were generated for over 7'000 inorganic metals. We also computed de Haas-van Alphen frequencies associated with each FS, enabling direct comparison of our simulations with experiments. The procedure is fully automated using the AiiDA workflow engine [2]. Our database will be published openly online and browsable on the Materials Cloud MC3D section (https://mc3d.materialscloud.org).

[1] J. Qiao, G. Pizzi, N. Marzari, npj Comput Mater 9, 208 (2023)
[2] S. P. Huber et al., Scientific data 7, 1 (2020)

MM 31.10 Thu 17:30 H10

A systematic benchmark of G_0W_0 calculations — •Marc Thieme, Max Grossmann, Malte Grunert, and Erich Runge — Technische Universität Ilmenau, Ilmenau, Germany

Accurate and efficient ab initio electronic structure calculations of semiconductors and insulators are a prerequisite for building large, high-quality databases for machine learning (ML). However, the "optimal" choice (speed vs. accuracy) of the approximations used, i.e. the exchange-correlation (XC) functional for density functional theory (DFT) calculations or a particular many-body perturbation theory, remains unclear. A systematic benchmark of band gaps of solids using several different DFT XC functionals by Borlido et al [1,2] showed that hybrid functionals perform exceptionally well and seem to be the functionals of choice. The present study addresses the question of whether G_0W_0 calculations provide a sufficient increase in accuracy to justify their increased computational cost compared to simpler DFT calculations with hybrid functionals. We calculate the band gaps for about 300 materials using the G_0W_0 method starting from LDA/PBE DFT calculations. The deviations between G_0W_0 and experimental band gaps are systematically compared with those of the best hybrid functionals

[1] Borlido et al., J. Chem. Theory Comput. 15, 9 (2019)

[2] Borlido et al., npj Comput. Mater. 6, 96 (2020)

MM 31.11 Thu 17:45 H10

Machine Learning-Assisted Design of Magnetic Materials: Predicting Properties for not purely ternary $Nd_2Fe_{14}B$ — •Manuel Enns, Daniel Urban, Wolfgang Körner, and Christian Elsässer — Fraunhofer IWM, Wöhlerstraße 11, 79108 Freiburg, Germany

$Nd_2Fe_{14}B$-based hard-magnetic materials are widely used for strong permanent magnets. Their re-use and recycling after the end of the magnet's life cycle opens the question of the degradation of the magnetic properties due to the incorporation of unintentional impurity elements originating from the recycling procedures. In this talk, we present a data-mining and machine-learning (ML) approach using kernel-based learning methods to predict the influence of impurity atoms in $Nd_2Fe_{14}B$-based materials. The magnetic-property data used for training and testing the ML model were obtained by a combinatorial high-throughput screening (HTS) using density-functional theory calculations. We demonstrate that our ML approach can accurately predict the saturation magnetization, the uniaxial anisotropy constant, and the formation energy for $Nd_2Fe_{14}B$ with impurities added by recycling.

MM 32: Transport in Materials: Diffusion, Charge or Heat Conduction

Battery Materials, Effects of Defects

Time: Thursday 15:00–17:45 Location: H22

MM 32.1 Thu 15:00 H22

Kinetic analysis of lithium transport in silicon anode using operando optical microscopy — •Shihao Wei, Monica Mead, Yug Joshi, and Guido Schmitz — Institute of Materials Science University of Stuttgart, 70569 Stuttgart, Germany

The performance of silicon(Si) anodes in lithium(Li)-ion batteries is significantly influenced by the kinetics of Li insertion and migration, particularly at the phase boundaries formed during cycling. Traditional techniques, such as EIS, SIMS, and NMR, are limited in providing detailed kinetic information at internal phase boundaries. This study proposes a novel approach to measure Li migration across phase boundaries in Si-based anodes. First, reflectance spectroscopy is employed to examine the optical response of Si thin films sputtered onto copper current collectors at various charge states, revealing reversible electrochromic behavior and the effect of Li content on spectral characteristics. Based on this, operando optical microscopy is developed to track the lithiation front, by using SU-8 photoresist as a patterning tool. The lithiation process is predominantly governed by diffusion-controlled parabolic growth, with minimal evidence of interface-controlled linear growth. Interestingly, applying the same method during delithiation, a significant slow-down of delithiation front appears. In addition, temperature-dependent diffusion behaviors are explored, quantified with an Arrhenius-like model. By altering the geometry of the photoresist patterns, the transport dynamics are analyzed under two distinct scenarios: a 1D semi-infinite planar configuration and a 2D finite circular configuration.

MM 32.2 Thu 15:15 H22

Crossing Boundaries? Probing Ion Conduction across Interfaces in Solid Electrolytes using Computational NMR Spectroscopy — •Tabea Huss[1], Federico Civaia[1], Simone Köcher[2,1], Karsten Reuter[1], and Christoph Scheurer[1,2] — [1]Fritz-Haber-Institut der MPG, Berlin — [2]Institute of Energy Technologies (IET-1), Forschungszentrum Jülich GmbH

Grain boundaries are critical, yet poorly understood factors affecting ion transport in solid-state electrolytes. The spin-alignment echo (SAE) nuclear magnetic resonance (NMR) experiment is a versatile tool to study the manifold transport processes of quadrupolar ions in these solid state materials. However, assigning the measured decay coefficients to physical transport phenomena often proves to be challenging. We have previously demonstrated that we can replicate the SAE experiment for bulk materials using a multi-scale machine learning framework.[1] This framework simulates both the atomic structure and dynamics of solid-state systems, along with generating solid state NMR observables. Our approach has already allowed us to predict electric field gradients over molecular dynamics trajectories and use them to compute decay constants that align with ion hopping times in bulk lithium thiophosphates. In this work, we extend our methodology to explore ion transport in grain boundary structures of the solid-state electrolyte $Li_{10}GeP_2S_{12}$. We extract SAE time constants and differentiate among various decay processes, advancing another step towards direct comparability with experimental results.

[1] A. F. Harper *et al.*, Faraday Discuss., (2024).

MM 32.3 Thu 15:30 H22

Theoretical Investigation of Electron Transport in the $LiMnPO_4$ Battery Material — •Franz Winkler[1,2] and Harald Oberhofer[1,2] — [1]University of Bayreuth — [2]Bavarian Center for Battery Technologies

Developing better batteries and thus battery materials is a crucial step in humanity's urgent energy transition. Thereby, theory can play an important role in characterizing and understanding the properties of the involved materials. In this contribution we present our work on $LiMnPO_4$ which exhibits some desirable properties such as a high energy density and a high potential and thus operating voltage. However, its adoption is hampered by a bad electronic conductivity.

Using electronic density functional theory (DFT), we compute the parameters of conductivity for both band- and polaronic hopping transport, to identify possible bottlenecks and thus possible future improvements of the material. For this we consider both the paramagnetic and antiferromagnetic configuration of $LiMnPO_4$. Due to the well known failures of plain semi-local DFT to represent both localized polaronic configurations and complex spin structures, we thereby use Hubbard-corrected DFT for the bulk of our calculations and range-separated hybrid DFT as a reference. Improvements suggested by our theoretical results can then help experimental collaborators to establish synthetic routes towards more efficient battery materials.

MM 32.4 Thu 15:45 H22

Lithium transport in Lithium Manganese Oxide as a function of temperature, concentration and grain size measured by operando optical microscopy — •Monica Mead[1], Yug Joshi[2], and Guido Schmitz[1] — [1]Institut für Materialwissenschaft, Universität Stuttgart, Heisenbergstr.3, 70569 Stuttgart — [2]Max-Planck-Institut für Nachhaltige Materialien, Max-Planck-Straße 1, 40237 Düsseldorf

Common methods for the determination of diffusion coefficients in electrode materials require critical interpretation, as their formal derivations rely on restrictive assumptions (e.g. galvanostatic/potentiostatic intermittent titration technique (G/PITT), electrochemical impedance spectroscopy (EIS), cyclic voltammetry (CV)). Alternatively, an optical method for studying ion transport in battery electrodes through operando microscopy can be applied. Here, the measurement of diffusion coefficients is done on thin films in lateral diffusion geometry and is based on an optical response upon ion intercalation. This allows measuring the diffusion coefficient as a function of temperature, concentration and grain size. In this work, diffusion of Li ions in Lithium Manganese Oxide (LMO) is studied by operando microscopy. The temperature dependence of the diffusion coefficient, providing the activation energy via the Arrhenius relation, and the diffusion coefficients for the bulk/grain boundaries of LMO can be determined. Additionally, it is possible to find the concentration dependence by an inverse Boltzmann-Matano method on concentration profiles derived from the intensity profiles along the diffusion direction.

MM 32.5 Thu 16:00 H22

Charge Transport Simulation in the High State-Of-Charge using Kinetic Monte Carlo — •Roya Ebrahimi Viand, Chiara Panosetti, Christoph Scheurer, Karsten Reuter, and Sebastian Matera — Fritz-Haber-Institut der MPG, Berlin

Understanding charge transport in solids is crucial for improving energy storage systems such as lithium-ion batteries. The diffusion of particles in solid materials typically involves rare transitions between low-energy sites, making kinetic Monte Carlo (kMC) an effective tool for studying the long-time dynamics. To address the computational challenges posed by long-range Coulomb interactions, we utilize fast rules for updating the process rates at each kMC step. We investigate ion transport on an isotropic rectangular lattice as well as in lithium graphite structures at high states of charge. We find that small changes in the ion concentration can significantly influence ion mobility, depending on temperature and dielectric response. This happens near stoichiometric concentrations, where the ions freeze in a Coulomb superlattice where effective motion is energetically uphill. Introducing defects or excess ions then opens effective pathways for diffusion. Finally, we discuss the possibility of multiple quasi-stationary states manifesting in different mobilities under the same applied conditions and concentrations.

15 min. break

MM 32.6 Thu 16:30 H22

Electrical characterization of the gate length dependence in graphene field-effect transistors — •Daniel Nickel[1], Daniele Capista[1], Rasuole Lukose[1], Christian Wenger[1,2], and Mindaugas Lukosius[1] — [1]IHP - Leibnitz Institute for High Performance Microelectronics, Im Technologiepark 25, 15236 Frankfurt (Oder), Germany — [2]BTU Cottbus Senftenberg, Platz der Deutschen Einheit 1, 03046 Cottbus, Germany

Integrating graphene into silicon complementary metal-oxide semiconductor technology for electronic and optoelectronic applications holds great promise but faces challenges such as limited graphene mobility. This work addresses this limitation by using graphene field-effect transistors (GFETs) to analyze the influence of fabrication parameters on the electrical properties of graphene and to investigate the gate length dependence of sheet mobilities at $T = 300$ K. The GFET devices are fabricated with a wolfram back-gate on a 200 mm SiO_2/Si wafer, transferring chemical vapor deposition-grown graphene, patterning it, and forming graphene channel contacts with Pd/Au and Ni. The Dirac point is well detected in electrical measurements, indicating the transition between p- and n-type conduction. Graphene mobility is evaluated using the transconductance method and total resistance fit, revealing peak mobilities of $\mu_p = 715$ cm^2/Vs for the p-branch and $\mu_n = 986$ cm^2/Vs for the n-branch, with dependencies on channel length and contact metals used. Funding was provided by the EU's Horizon 2020 research and innovation program under the Graphene Flagship grant agreement no. 101189797.

MM 32.7 Thu 16:45 H22

Structural and electronic impact of defective sites and their effects on the thermoelectric properties of scandium nitride thin films — •Luigi Cigarini, Urszula Danuta Wdowik, and Dominik Legut — IT4Innovations, VŠB Technical University of Ostrava, 17. listopadu 2172/15, 708 00 Ostrava-Poruba, Czech Republic

The Landauer model provides a theoretical tool to understand the electronic transport mechanisms that deeply govern at the atomic scale the thermoelectric conversion of interesting materials. Transition metals nitrides are currently studied for potential applications in energy conversion. Modeling the effects on electronic transport that result from the electronic and structural modifications produced by oxygen impurities and spatial vacancies in scandium nitride (ScN), we propose a theoretical interpretation for new experimental results revealing a strong dependence of the thermoelectric properties of ScN thin films on procedural changes during their fabrication. We find that the thermoelectric properties of ScN are actually decisively determined by the structural and electronic factors caused by the presence of these defects or impurities. Evaluating to what extent these material's overall properties are influenced by these features necessarily requires a theoretical approach. This is particularly true as the presence of oxygen, which proves to be a decisive factor, is extremely difficult to control in standard fabrication processes and experimental conditions. The results presented in this contribution demonstrate the potential of this theoretical approach in studying the thermoelectric properties of these materials uncovering future strategies for improvement.

MM 32.8 Thu 17:00 H22

Helium Interaction with Atomic Level Defects in TungstenStudied by Positron Annihilation Spectroscopy — •Vassily Vadimovitch Burwitz[1,2], Annemarie Kärcher[1,3], Maik Butterling[4], Eric Hirschmann[4], Emma Huntley[2], Adrian Langrehr[1,2], Maciej Oskar Liedke[4], Lucian Mathes[1,2], Thomas Schwarz-Selinger[3], Christoph Springl[1,2], Monia Vadrucci[5,6], Andreas Wagner[4], and Christoph Hugenschmidt[2] — [1]TU München, School of Natural Sciences, Physikdepartment — [2]TU München, MLZ — [3]MPI für Plasmaphysik, Garching — [4]HZDR, Institute of Radiation Physics — [5]ENEA, Development of Particle Accelerators and Medical Applications, Frascati (RM), Italy — [6]Italian Space Agency, Science and Innovation Directorate, Rome

Understanding the type and evolution of lattice defects in tungsten (W) is of interest in nuclear fusion materials research. We therefore investigated W(111) mono-crystals by positron annihilation Doppler-broadening spectroscopy (DBS) and positron annihilation lifetime spectroscopy (PALS). Both complementary methods are sensitive tools for the examination of the defect type and concentration. The literature currently lacks conclusive experimental work regarding the influence of He decoration of vacancies on PAS. We therefore irradiated samples by 4.5 MeV electrons to different damage levels in order to specifically produce mono-vacancies in W. We will present DBS and PALS measurements, both performed with a slow positron beam, before and after plasma loading with 50 eV He ions. The implantation energy is chosen low enough to prevent displacement damage.

MM 32.9 Thu 17:15 H22

Formation energies and charge transition levels of charged point defects in Hematite — •Hao Chen, Christoph Freysoldt, Mira Todorova, and Jörg Neugebauer — Max-Planck-Institut für Nachhaltige Materialien GmbH, Düsseldorf, Germany

Hematite (Fe_2O_3), an iron oxide fundamental to the process of iron ore reduction, exhibits rich defect physics and off-stoichiometric features, as iron can occur as either Fe^{3+} and Fe^{2+}. Charged point defects and the associated Fe^{2+}/Fe^{3+} transitions play an important role in phenomena such as thermodynamic stability, phase transitions between iron oxides, and electronic structure modulation. In order to correctly account for these effects in the prediction of defect equilibria, phase diagrams, diffusion, and related properties, a robust framework for understanding defect thermodynamics and constructing a comprehensive defect model at the ab initio level is essential. Here, we employ DFT+U as an efficient tool for studying strongly correlated systems. In view of the delocalization error of standard functionals, DFT+U is crucial to investigate Fe^{2+} ions as distinct species. Moreover, it systematically opens the band gap of the bulk iron oxides. Since Hubbard U parameter has a direct influence on the band structure and Fe-related defect states in the band gap, we investigate the impact of U values on the computed formation energies of vacancies and interstitials. Our results show that the defect formation energies have a surprisingly weak dependence on U, thus allowing reliable predictions. We analyze the electronic structures of the defects in detail to uncover the underlying physical mechanisms.

MM 32.10 Thu 17:30 H22

Contribution of damped collective modes to thermopower in the strange metal phase of cuprates — •Giovanni Mirarchi[1], Sergio Caprara[2,3], Carlo Di Castro[2], Götz Seibold[4], and Marco Grilli[2,3] — [1]Institute of Theoretical Physics and Astrophysics, University of Würzburg, Am Hubland, 97074 Würzburg, Germany — [2]Dipartimento di Fisica, Sapienza Università di Roma, P. le Aldo Moro 5, 00185 Roma, Italy — [3]ISC-CNR, Unità di Roma Sapienza, P. le Aldo Moro 5, 00185 Roma, Italy — [4]Institut für Physik, BTU Cottbus-Senftenberg - PBox 101344, D-03013 Cottbus, Germany

The strange-metal behavior, which is still an unsolved problem in condensed matter physics, is typically signaled by anomalies in thermodynamic and transport properties, including the famous linear-in-temperature resistivity [1]. The best-known case of strange-metal behavior in literature is that of high-temperature superconducting cuprates, whose strange-metal phase seems to always be accompanied by some kind of dynamical charge order [2]. Based on the experimental evidence of damped short-ranged charge density collective modes in the strange-metal phase of cuprates [3], we propose a scenario in which these collective modes can affect the phenomenology of this phase by interacting with electrons and by directly contributing to thermodynamics and transport [4]. In this talk, the concept of heat current in the presence of damping is discussed and used to describe the Seebeck effect in cuprates through a mechanism analogous to phonon drag. [1] Nat. Phys. 15, 142-147 (2019). [2] Science 337, 821 (2012). [3] Science 365, 906-910 (2019). [4] Commun. Phys. 5, 10 (2022).

MM 33: Invited Talk: P. Sonnweber-Ribic

Time: Friday 9:30–10:00 Location: H10

Invited Talk MM 33.1 Fri 9:30 H10

Fatigue in steels: Micromechanical modelling of cyclic damage — •Petra Sonnweber-Ribic[1], Alexandra Stark[1], and Christian Elsässer[2] — [1]Robert Bosch GmbH, Renningen — [2]Fraunhofer-Institut für Werkstoffmechanik IWM, Freiburg

Fatigue is a common phenomenon in engineering structures and can lead to unexpected failures, especially in critical components such as aircrafts, trains, and automotive parts. Understanding the mechanisms behind fatigue is crucial for ensuring the safety and reliability of these structures. A specific challenge of fatigue lies in the difficulty of external detection, as the initial stages of fatigue damage manifest as highly localized processes within specific microstructural domains.

The micromechanical modelling offers a method for predicting fatigue properties and achieving a more profound comprehension of damage and relevant micromechanical parameters. Initially, this is based on the representation of the underlying microstructure of the material and the description of local plastic deformation using the crystal plasticity method. This approach has been successfully employed in industrial environment to assess the role of different metallographic phases in relation to local cyclic damage, among other applications.

Subsequently, this methodology can be enhanced by integrating a hydrogen diffusion approach and advanced damage models to consider the influence of hydrogen on fatigue damage mechanisms. The relevance of different influencing factors is analyzed based on selected examples.

MM 34: Development of Calculation Methods

Atomic Structure, Quantum Effects

Time: Friday 10:15–12:15 Location: H10

MM 34.1 Fri 10:15 H10

Enhancing 3D Volume Reconstruction in Atom Probe Tomography through Curvature-Based Tip Shape Analysis — Sebastian Eich and •Guido Schmitz — Department for Materials Physics, Institute for Materials Science, University of Stuttgart

Atom Probe Tomography (APT) provides chemical analysis of nanometric volumes with single-atom sensitivity in 3D. Traditionally, reconstruction assumes a hemispherical tip shape, which can lead to significant distortions, especially due to local magnification effects.

Instead of relying on in-situ correlative microscopy, we propose a numerical method to extract the emitter shape from the event density statistics on the 2D detector plane. This method is based on the fundamental relationship between event density and the local Gaussian curvature of the tip surface, with no mathematical restrictions other than convexity. By knowing the curvature and assuming suitable boundary conditions, the surface profile can be uniquely reconstructed, bypassing the need for a hemispherical assumption.

The method is implemented as an easy-to-use Python module, which will be demonstrated using various simulated and experimental datasets involving complex tip shapes. This approach significantly reduces the local magnification effects at material interfaces with contrasting evaporation thresholds and is expected to improve the accuracy of atom probe reconstructions.

MM 34.2 Fri 10:30 H10

Sum frequency generation from real-time simulation in 2D crystals — •Mike Nico Pionteck[1], Myrta Grüning[2,3], Simone Sanna[1], and Claudio Attaccalite[3,4] — [1]Institut für Theoretische Physik and Center for Materials Research (LaMa), Justus-Liebig-Universität Gießen, Germany — [2]School of Mathematics and Physics, Queen's University Belfast, United Kingdom — [3]European Theoretical Spectroscopy Facilities (ETSF) — [4]CNRS/Aix-Marseille Université, Centre Interdisciplinaire de Nanoscience de Marseille UMR 7325 Campus de Luminy, France

Sum and difference frequency generation (SFG, DFG) are powerful experimental techniques which involve the interaction of two laser with frequency ω_1 and ω_2, generating an output beam with frequency $\omega = \omega_1 \pm \omega_2$ as second-order nonlinear response. These techniques are widely used to study 2D materials, providing complementary insights to those obtained from infrared and Raman spectroscopy.

We present an implementation of SFG and DFG within the Yambo code [1], based on real-time time-dependent adiabatic GW (TD-aGW). To account for local field effects and electron-hole interactions, our approach reduces to the Bethe-Salpeter equation (BSE) in the linear limit regime. We demonstrate this framework by calculating SFG and DFG signatures in h-BN and MoS_2. Furthermore, the method enables the extraction of higher-order response functions (e.g. TPA). This work establishes a first-principles approach to nonlinear optics, enabling investigations of optical responses of bulk materials with high versatility. [1] D. Sangalli *et al.*, J. Phys. Condens. Matter **31**, 325902 (2019).

MM 34.3 Fri 10:45 H10

Ab initio calculations of longitudinal electrical conductivity using a Wannier-based coherent potential approximation — •Shota Namerikawa and Takashi Koretsune — Department of Physics, Tohoku University, Sendai, Japan

We present a longitudinal electrical conductivity calculation method for disordered alloys applicable from a wide range of density functional theory (DFT) codes based on the first-principles Wannier-based coherent potential approximation (Wannier-CPA). For evaluation of electrical conductivity, we employ two complementary methods; the Kubo-Greenwood formula and numerical analytic continuation of the current-current correlation function. We apply the developed method to Ag-Pd alloys and find that the results obtained by the Wannier-CPA reasonably reproduce previous studies by the well-established CPA implementation based on the Korringa-Kohn-Rostoker Green*s function method (KKR-CPA).

MM 34.4 Fri 11:00 H10

Ab-initio-based analysis of phonon contributions to negative thermal expansion of α-tin — •Petr Čípek[1,2], Jana Pavlů[2], Martin Friák[1], and Alena Michalcová[3] — [1]Inst. Phys. Mater., Czech Acad. Sci., Brno, Czech Rep. — [2]Dept. Chem., Masaryk Uni., Brno, Czech Rep. — [3]Dept. Met. Corr. Eng., Uni. Chem. Technol.

Prague, Czech Rep.

We applied quantum-mechanical calculations to investigate tin's thermodynamic and dynamic stability in its various allotropic forms. Focusing specifically on the a-Sn, our results showed a negative thermal expansion within the temperature range from T = 0 K to T = 45 K. No similar phenomenon appears in spectra of other allotropic modifications of tin. That means that the origin of this behaviour is connected to the diamond structure of alpha tin. We investigated the behaviour of the Grüneisen constant of a-tin in reciprocal space to explain the causes of this phenomenon. There are interesting temperature-dependent contributions of individual phonon modes from different k-points in the reciprocal space. In particular, these contributions are negative at all studied temperatures for the k-points around k-point X (0, 0, 0.5) and positive around k-point Γ (0, 0, 0). Negative thermal expansion of a-Sn at low temperatures is thus related to the behaviour of phonons around k-points X, M and N.

MM 34.5 Fri 11:15 H10

Bayesian Uncertainty Estimates for Spin-Component-Scaled Second-Order Møller-Plesset Perturbation Theory — •Elisabeth Keller and Johannes Margraf — Universität Bayreuth, Bayreuth, Germany

Spin-component-scaled second-order Møller-Plesset perturbation theory (SCS-MP2) improves upon MP2 by separately scaling the same-spin and opposite-spin MP2 contributions, achieving near coupled cluster (CCSD(T)) accuracy in some applications. However, the optimal scaling parameters vary by target domain, limiting the transferability of any given SCS-MP2 parameterization. To address this limitation, we employ a Bayesian multilevel linear regression model to obtain a robust parameterization for SCS-MP2, termed BSCS-MP2, predicting various energetic properties, including total, atomization, reaction, and non-covalent interaction energies. Additionally, the Bayesian model provides credible intervals to quantify the uncertainty of the BSCS-MP2 energy predictions. We evaluate how these uncertainty estimates adjust to data quality and model complexity, and assess their robustness for out-of-sample inference.

15 min. break

MM 34.6 Fri 11:45 H10

pyTTN, an open source toolbox for Quantum Dynamics simulations using Tree Tensor Network states — Lachlan Lindoy, •Daniel Rodrigo-Albert, Yannic Rath, and Ivan Rungger — National Physical Laboratory, Teddington, TW11 0LW, United Kingdom

The simulation of large-scale dissipative quantum systems is a significant challenge arising in several areas of physics and chemistry. In this talk we will discuss pyTTN, our recently developed software package for simulating dynamical properties of open quantum systems. This package makes use of Tree Tensor Network (or equivalently, Multi-Layer Multi-Configuration Time-Dependent Hartree) based representations of the state vector, and features both single- and multi-set ansätze, as well as adaptive bond dimension through subspace expansion techniques. The software has been designed with a focus on performance and ease of setup of new models and wavefunction topologies, including simple preparation of zero- and finite-temperature calculations with general bosonic, fermionic, and spin Hamiltonians. We will demonstrate the capabilities of the package with both unitary dynamics and non-unitary pseudomode-based approaches for the simulation of Anderson impurity models.

MM 34.7 Fri 12:00 H10

Spectral properties from an efficient analytical representation of the GW self-energy within a multipole approximation — •Dario Alejandro Leon[1], Kristian Berland[1], and Claudia Cardoso[2] — [1]Norwegian University of Life Sciences, As, Norway — [2]S3 Centre, Istituto Nanoscienze, CNR, Modena, Italy

We propose an efficient analytical representation of the frequency-dependent GW self-energy via a multipole approximation (MPA-Σ). Similar to the earlier developed multipole approach for the screening interaction W (MPA-W) [Phys. Rev. B 104, 115157 (2021)], the multipole-Padé model for the self-energy is interpolated from a small set of values evaluated numerically in the complex frequency plane. As for MPA-W , we show that an appropriate choice of the frequency sampling is paramount to guarantee computational efficiency and high level of accuracy in the description of the self-energy. Crucially, MPA-Σ enables a multipole representation for the interacting Green's function G (MPA-G), providing straightforward evaluation of all the spectral properties. Combining the MPA-W and MPA-Σ schemes considerably reduces the cost of full-frequency self-energy calculations, especially when targeting spectral band structures in a wide energy range. We validate the MPA-Σ approach in bulk Si, Na and Cu, monolayer MoS2, the NaCl ion-pair and the F2 molecule, as prototypical semiconducting and metallic materials of different dimensionality. Moreover, toy MPA-Σ models with one and two poles and their corresponding MPA-G solutions, are used to examine the quasiparticle picture in different situations.

MM 35: Transport in Materials: Diffusion, Charge or Heat Conduction

Diffusion

Time: Friday 10:15–11:45 Location: H22

MM 35.1 Fri 10:15 H22

Influence of second phase precipitation on bulk diffusion of Ni in the CoFeMnNiV high-entropy alloy — •Aditya Burla[1], Mohan Muralikrishna Garlapati[1], Aditya Srinivasan Tirunilai[2], Guillaume Laplanche[2], Gerhard Wilde[1], and Sergiy V Divinski[1] — [1]Institut für Materialphysik, Universität Münster, 48149 Münster, Germany — [2]Institut für Werkstoffe, Ruhr-Universität Bochum, 44780 Bochum, Germany

High-entropy alloys (HEAs), or multi-principal element alloys represent a new class of metallic materials that offer tremendous opportunities for advancing materials science due to their vast compositional space and exceptional properties. While tracer diffusion and sigma phase precipitation kinetics in the Co-Cr-Fe-Mn-Ni system have been widely studied, the interaction between the two has received limited attention. The present work focuses on an equiatomic CoFeMnNiV HEA, in which Vanadium is known to have a strong tendency to stabilize the sigma phase. Therefore, this element promotes its precipitation in the CoFeMnNiV alloy, particularly at temperatures below ~1080°C, even after short anneal times of just 1 h in the fully recrystallized state. In this study, bulk diffusion of Ni is investigated using the radiotracer technique. A strong impact of sigma phase precipitation on the self-diffusion kinetics was discovered and analyzed. The obtained tracer diffusivities follow an Arrhenius-type relationship when estimated in the stable microstructures, whereas concurrent precipitation enhances the tracer diffusion rates.

MM 35.2 Fri 10:30 H22

Investigation of lateral hydrogen diffusion in polycrystalline molybdenum trioxide thin films — •Tim K. Hecker, Martin Becker, and Peter J. Klar — Institute of Experimental Physics I and Center for Materials Research, Justus Liebig University Giessen, Giessen, Germany

Molybdenum trioxide thin films were prepared by RF sputter deposition exploring a wide range of growth parameters. To characterise the thin films, electrochemical, Raman, and XRD experiments were conducted. In order to gain a deeper understanding of the diffusion of hydrogen in these thin films, the samples were microstructured with a PMMA film in a way that restricts the contact surface with the electrolyte to a narrow stripe-like gap. This enables the lateral diffusion of hydrogen beneath the PMMA film to be studied using a transmission experiment, making use of the electrochromic properties of molybdenum trioxide. This increases the accessible spatial and temporal scale by several orders of magnitude, significantly improving the spatial and temporal resolution of the in-situ transmission measurement. Spatially resolved transmission measurements in the wavelength range of 633±55 nm demonstrate that the investigated diffusion is dependent on the hydrogen concentration. The results are also supported by a spatially and temporally resolved diffusion simulation. Furthermore, the measurement method presented here is universally applicable to electrochromic thin film samples.

MM 35.3 Fri 10:45 H22

Diffusion and activation energies of hydrogen and its isotopes in boron structure — •Bianca Solomonea[1,2], Calin Pantis-Simut[2,3], Mihaela Cosinschi[2,3], Paul Dinca[1], Corneliu Porosnicu[1], and George Nemnes[2,3] — [1]National Institute for Laser, Plasma and Radiation Physics (INFLPR), Atomiştilor Street 409, 077125 Măgurele, Ilfov, Romania — [2]Faculty of Physics, University of Bucharest, Atomistilor 405, Magurele-Ilfov 077125, Romania — [3]Horia Hulubei National Institute for Physics and Nuclear Engineering, Reactorului 30, Magurele-Ilfov 077125, Romania

The retention and release of hydrogen isotopes in plasma-facing materials (PFM) is a critical concern for the ITER project. The decision to construct the Tokamak reactor as a fully tungsten-based machine presents challenges regarding plasma ignition and stability, particularly due to impurities in the working gases. Boronization is applied to retain impurities by forming covalent bonds with oxygen and nitrogen. This study uses ab initio calculations via Density Functional Theory (DFT), molecular dynamics (MD), and the nudged elastic band (NEB) method in the SIESTA code to examine boron structures in crystalline and amorphous forms. Activation energies for trapping, detrapping, and diffusion processes are determined. Given the difficulty of defining hydrogen-isotope diffusion in boron structures, and its importance for retention and desorption in redeposited or co-deposited layers of the PFM, we focus on identifying the potential diffusion trajectories of hydrogen within the boron structure. This includes mapping a potential landscape and locating local minima and saddle points.

MM 35.4 Fri 11:00 H22

Diffusion behavior of Li ions in crystalline and amorphous Li-Zr-O and Li-Nb-O phases — •Daniel Mutter[1], Diego A. Pantano[2], Christian Elsässer[1], and Daniel F. Urban[1] — [1]Fraunhofer IWM, Wöhlerstraße 11, 79108 Freiburg, Germany — [2]TotalEnergies OneTech, 2 place Jean Millier, 92400 Courbevoie, France

Li containing transition metal oxides are known as good ionic conductors. Performing classical molecular dynamics simulations with a Morse potential model based on the Bond Valence method, the diffusion behavior of Li ions is investigated in crystalline and amorphous phases with the stoichiometries Li_2ZrO_3 and $LiNbO_3$. The diffusivities are obtained from a statistical Arrhenius analysis of mean square displacement curves at different temperatures. The crystalline phase of Li_2ZrO_3 exhibits two well-defined migration mechanisms: vacancy-mediated migration is dominant below and a collective site exchange of Li ions above a crossover region between about 1700 and 1800 K. The latter mechanism, which is related to the formation of Frenkel pair defects and subsequent rotation of Li-Li pairs, also prevails in the amorphous phases with a strongly reduced activation energy. This is explained by a smaller equilibrium separation of Li ions in the amorphous phase than in the crystal structure. The demonstrated methodology and the discussed results shed light on a hitherto rarely described diffusion mechanism in ionic metal-oxide materials relevant for ion-battery applications.

MM 35.5 Fri 11:15 H22

Ag bulk and grain boundary diffusion in AlCoCrFeNi2.1 compositionally complex alloy — •Heng Zhang, Mohan Muralikrishna Garlapati, Sergiy V Divinski, and Gerhard Wilde — Institute of Materials Physics, University of Munster, Wilhelm-Klemm-Str. 10

Bulk and grain boundary diffusion of Ag in a eutectic Al-Co-Cr-Fe-Ni multi-principal element system is measured using the radiotracer technique and applying the 110Ag radioisotope. An equilibrium microstructure was produced by rotary forging and annealing of cast and homogenized initial casting ingot material. Ag diffusion is measured in the temperature interval from 673K to 1373K accounting for volume (at high temperatures) and short-circuit (at moderate and low temperatures) diffusion contributions. In the present case, interphase boundaries can potentially contribute in addition to grain boundaries to the short-circuit diffusion. The grain- and interphase-boundary diffusion experiments were performed in the B-type kinetic regime based on Harrison's classification. The results are analyzed with respect to constituent phases (FCC and B2) and different interface types. The contribution of interphase boundary diffusion is analyzed in detail.

MM 35.6 Fri 11:30 H22

Mechano-chemical coupling induced by Co grain boundary diffusion in SIGMA5(310) Cu bicrystals — •Esakkiraja Neelamegan[1], Anoosheh Akbari[1], Hui Ding[2], Harald Rösner[1], Daniel Gaertner[1], Christian Liebscher[2,3], Gerhard Wilde[1], and Sergiy Divinski[1] — [1]Institute of Materials Physics, University of Münster, Münster-48149 Germany — [2]Max-Planck-Institut für Sustainable Materials, Düsseldorf, Germany — [3]Faculty of Physics and Astronomy, Ruhr University Bochum, Bochum, Germany

Grain boundary diffusion of 57Co in pure copper SIGMA-5(310)[001] bicrystals is investigated using the radiotracer technique. Experiments are conducted under both the type-B and type-C kinetics regimes, as classified by Harrison. By varying the amount of applied 57Co tracer solution, characteristic changes in the shape of the penetration profiles are observed and attributed to Co segregation induced changes of the grain boundary structure. The structural changes due to the Co addition are examined by scanning transmission electron microscopy. The elastic strains near the grain boundary are measured using nano-beam diffractions with a nanometer resolution. The Co-induced variations of the GB structure provide an intriguing picture, particularly when considering their influence on the diffusion behaviour in the presence of deliberately introduced solute atoms.

MM 36: Mechanical Properties

Nanomaterials and Alloys

Time: Friday 10:15–13:00 Location: H23

MM 36.1 Fri 10:15 H23

STEM investigation of early precipitation reactions in Al-Cu alloys — •Johannes Berlin and Ferdinand Haider — Chair for Experimental Physics I, University of Augsburg, Universitätsstraße 1, 86159 Augsbur

Due to their excellent strength-to-weight ratio, heat-treatable Al-Cu alloys have been widely used since their invention. Although the occurring precipitates in naturally aging aluminium alloys are well known, the very early stages of formation mechanisms still are a topic of ongoing research. Scanning transmission electron microscopy is used to investigate the influence of different parameters, such as thermal history and effects of microalloying, on early-stage precipitate formation and transformation in Al. Due to their strong binding potential to quenched in vacancies even a few hundred ppm of trace elements such as tin and indium can alter the natural aging process drastically. Even after prolonged natural ageing, a slight increase in temperature can lead to drastic changes in precipitation size and densitiy inthese materials. This proves a long-lasting supersaturation of the material with vacancies. Additionally, these results are compared to the measurements of hardness, DSC and electrical resistance.

MM 36.2 Fri 10:30 H23

Surface structure and reactivity of Aluminium alloys studied by DFT — •Zhengqing Wei[1], Inna V. Plyushchay[2], Nebahat Bulut[1], Florian Lehmann[3], Maik Gude[3], Julia Hufenbach[4,5], and Sibylle Gemming[1,6] — [1]Inst. Physics, TU Chemnitz, Germany — [2]Natl. Taras Shevchenko University of Kyiv, Ukraine — [3]ILK, TU Dresden, Germany — [4]IFW Dresden, Germany — [5]Inst. Materials Science, TU-BA Freiberg, Germany — [6]MAIN Center, TU Chemnitz, Germany.

Classically, the mechanical properties of alloys are attributed to the action of stress fields around defect sites and to their combined influence on the overall elastic moduli. The present study employs first-principles modeling to include also changes of the electronic structure and investigate the bonding, stability, and reactivity changes around impurities in the bulk and at surfaces. We focus on Al alloys with low amounts of substitutional Mg, Zr, and Si atoms. The results indicate that the electron density changes mostly within the first coordination sphere around the impurity, the bond lengths vary locally within few percent, and there exists a thermodynamic driving force for most elements to diffuse to or near surfaces or interfaces. Stable 2D surface alloy compositions in part differ from the bulk phase and exhibit an element-specific reactivity with air and polymer coatings. Modeling the adsorption of oxygen, nitrogen and the PEEK polymer from first principles gives access to modified local potentials for the classical modeling of large-scale surface and interface areas (tu-dresden.de/ing/forschung/Graduiertenkollegs/grk2868#intro).

MM 36.3 Fri 10:45 H23

Active learning-based interatomic potential for investigating mechanical properties of Al-Mg-Zr alloys — •Lukas Volkmer, Leonardo M. Sandonas, Gianaurelio Cuniberti, and Markus Kästner — Technische Universität Dresden

The unique properties of aluminum-based alloys, such as low density, high specific strength, and excellent resistance to oxidation and corrosion, enable the design of advanced metamaterials. In this work, we theoretically investigate the effect of alloying aluminum with magnesium and zirconium on its thermodynamic and mechanical properties. Since exploring the vast chemical compound space of these alloys through Density Functional Theory (DFT) calculations is computationally prohibitive, we developed a scalable and transferable machine learning interatomic potential (MLIP) capable of accurately calculating diverse properties of Al-Mg-Zr alloys. The MLIP was trained using an active learning technique based on ab initio molecular dynamics simulations, Bayesian statistics, and kernel ridge regression. This methodology ensures that the MLIP captures the effects of alloying concentration and atomic configurations up to the solubility limit, providing access to highly accurate physicochemical properties of a wide range of Al-based alloys at a reasonable computational cost. We expect this approach to enable efficient phase space exploration, offering a robust tool for designing advanced Al-based alloys with optimized properties.

MM 36.4 Fri 11:00 H23

Phase identification by Raman Spectroscopy on pre-oxidized AISI 316L-MgO composite produced by Spark Plasma Sintering — •Julia Richter[1], Mahnaz Mehdizadehlima[2], Cameliu Himcinschi[1], and Jens Kortus[1] — [1]TU Bergakademie Freiberg, Institut für Theoretische Physik, Leipziger Straße 23, D-09599 Freiberg — [2]TU Bergakademie Freiberg, Institut für Werkstoffwissenschaft, Gustav-Zeuner-Straße 5, D-09599 Freiberg

Re-usage, recycling and upcycling of MgO-C refractories as they are widely used in the steel industry are crucial for resource efficiency. Our upcycling concept is aimed at steel-MgO composite anodes for application in the extraction of aluminum by fused-salt electrolysis. The composite anode material is produced by Spark Plasma Sintering based on 60 vol.% AISI 316L steel powder and 40 vol.% MgO. In this stage of development, the raw material is fused fresh MgO instead of recyclate as a proof of concept. Pre-oxidation treatment of the developed composite is intended to enhance the material's corrosion resistance in the aggressive environment of molten cryolite during application. In order to gain a better understanding of the oxidation behavior at different temperatures, phase identification is required. For this purpose, Raman spectroscopy as a sensitive, non-destructive, non-contact method is employed complementary to other investigative techniques; e.g., Scanning Electron Microscopy.

MM 36.5 Fri 11:15 H23

Atomic Cluster Expansion for Ag-Au-Pd alloys — •Yanyan Liang, Matous Mrovec, Yury Lysoroskiy, and Ralf Drautz — ICAMS, Ruhr-Universität Bochum, Germay

Ternary alloys of Ag-Au-Pd are of technological importance in catalysis and electrical applications. However, the system lacks reliable and efficient interatomic potentials capable of accurately describing structural and thermodynamic properties, particularly for investigating complex segregation and ordering phenomena in bulk systems and nanoclusters. In this work, we present an atomic cluster expansion (ACE) model parameterized for the Ag-Au-Pd system with quantum-level accuracy. We demonstrate that the ACE model provides an accurate description of fundamental properties, including structural stability and thermodynamics, not only for the elemental metals but also for their binary and ternary compounds. Furthermore, we highlight the wide applicability of the ACE model for large-scale atomistic simulations, enabling predictive modeling of complex phenomena.

15 min. break

MM 36.6 Fri 11:45 H23

Scalable fabrication and mechanical behavior of hierarchical nanoscale network nickel — •Ulrike Dette[1,2], Lukas Lührs[2], and Shan Shi[1,3] — [1]Research Group of Integrated Metallic Nanomaterials Systems, Hamburg University of Technology, 21073 Hamburg, Germany — [2]Institute of Materials Physics and Technology, Hamburg University of Technology, 21073 Hamburg, Germany — [3]Institute of Hydrogen Technology, Helmholtz-Zentrum Hereon, 21502 Geesthacht, Germany

The recent fabrication of mechanically robust two-level hierarchical nanoporous gold by two-step electrochemical dealloying has enabled the demonstration of enhanced mechanical properties and reduced density attributed to the structural hierarchy in the nanoscale network materials. This work aims to develop a new method for the scalable fabrication of low-cost hierarchical nanoscale network metals. Here, two- and three-level hierarchical network (HN) Ni samples are successfully prepared from Ni foams by a novel and simple alloying-dealloying method. Bulk three-level HN Ni samples are characterized by three well-defined strut/ligament sizes (160 μm, <10 μm and <10 nm) and a low density down to 0.06. In addition, we systematically perform mechanical studies on both two- and three-level HN Ni via macroscopic compression tests. We propose general scaling equations between mechanical properties and relative density for HN materials.

MM 36.7 Fri 12:00 H23

Transferable machine learning interatomic potential for Au nanoparticles — •Jovana Vlahović, Cem Sevik, and Milorad V. Milošević — University of Antwerp, Groenenborgerlaan 171, Antwerp, Belgium

Effective molecular dynamics and Monte Carlo simulations fundamentally depend on the accuracy of interatomic potentials, which define the potential energy surface as a function of atomic positions. This precision is essential for metallic nanoparticles (NPs), whose small size and diverse morphologies demand robust modelling. While classical empirical potentials offer computational efficiency, they often lack the necessary accuracy and density functional theory (DFT) calculations, though highly accurate, are computationally prohibitive for NPs with thousands of atoms. This work introduces a machine learning-based interatomic potential for Au NPs, trained on a compact dataset of bulk structures, surface slabs and NPs containing up to 55 atoms. Our training dataset includes a diverse set of atomic configurations with corresponding properties obtained from ab initio molecular dynamics calculations, which we use to train a Gaussian Approximation Potential (GAP) via Gaussian Process Regression. Parameter optimization was performed to maximize model accuracy, and LAMMPS validation tests demonstrated GAP performance against DFT benchmarks. In addition, transferability tests on larger NPs of various shapes reveal our GAP's robustness beyond the training set. Comparisons with an existing GAP model and the universal MACE potential underscore our model's improved accuracy and generalizability for Au NPs.

MM 36.8 Fri 12:15 H23

Scaling behavior of Poisson's ratio in hierarchical nanoporous materials — •Haonan Sun[1,2], Lukas Lührs[2], Wei-che Chang[3], and Shan Shi[1,3] — [1]Research Group of Integrated Metallic Nanomaterials Systems, Hamburg University of Technology, 21073 Hamburg, Germany — [2]Institute of Materials Physics and Technology, Hamburg University of Technology, 21073 Hamburg, Germany — [3]Institute of Hydrogen Technology, Helmholtz-Zentrum Hereon, 21502 Geesthacht, Germany

The recent fabrication of crack-free monolithic hierarchical nested network nanoporous gold allows the investigation of the benefits of hierarchy in the aspect of mechanical properties at the nanoscale. It has been demonstrated that hierarchical nanoporous gold (HNPG) can achieve a substantially reduced solid fraction and enhanced specific stiffness and strength compared with non-hierarchical nanoporous gold. However, the role of hierarchical structure on Poisson's ratio has not been investigated yet. In this work, mm-sized HNPG samples are made out of an Ag93Au7 master alloy by a dealloying-coarsening-dealloying method. We then explore the elastic and plastic Poisson*s ratios of HNPG by using digital image correlation during compression tests. Remarkably, a scaling law of the elastic Poisson's ratio in hierarchical nanoporous materials with respect to the solid volume fraction is proposed and excellently supported by our experiments. This work enriches the understanding on the relationship between mechanical properties and microstructure in hierarchical network materials at the nanometer scale.

MM 36.9 Fri 12:30 H23

Frenkel pair energetics in disordered solid solutions and implications for alkali feldspar diffusivity — •Alexander Gorfer, Rainer Abart, and Christoph Dellago — University of Vienna, Vienna, Austria

Predicting defect concentrations from the density of states (DOS) of formation energies in disordered materials has recently been formulated for vacancies in high entropy alloys. That methodology however does not translate to disordered ionic crystals as charged defects need to be paired up to ensure charge neutrality. Here, we present a general expression to predict the defect concentrations of Frenkel pairs in disordered ionic crystals out of the DOS of formation energies of both positively and negatively charged defects. To demonstrate its applicability we use a recently developed machine learning force field to calculate the DOS of formation energies for different states of (dis)ordering in alkali feldspar $(\mathrm{Na,K})\mathrm{AlSi_3O_8}$, an abundant mineral in the Earth's crust. Applying our expression to these DOS reveals a significant increase in the concentration of point defects in disordered ionic crystals as pairs of low formation energy defect states between the positively and negatively charged DOS can be identified. Implications for the diffusivity that controls the exsolution of alkali feldspars which is an important phenomenon in the formation of magmatic and metamorphic rocks are discussed.

MM 36.10 Fri 12:45 H23

Ferromagnetism at ambient temperature in Cantor and nanocomposite high-entropy alloys induced by severe plastic deformation — •Shabnam Taheriniya, Harald Rösner, and Gerhard Wilde — Universität Münster, Institut für Materialphysik, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany

In this study, single phase Cantor (CoCrFeMnNi) and nanocomposite high-entropy alloys (HEAs) (CoCrFeMnNi and HfNbTaTiZr) were processed using high-pressure torsion (HPT), subjecting the samples to a constant pressure of 9 GPa either as a single disk or stacked disks, with the top anvil rotating at 1 rpm at ambient temperature for up to 15 revolutions. Vibrating sample magnetometry (VSM) confirmed that HPT processing induces the development of ferromagnetic properties. The distribution and orientation of magnetic domains post-deformation were examined in detail using differential phase contrast scanning transmission electron microscopy (DPC STEM), analytical TEM and atom probe tomography (APT) analysis. Our study demonstrates that HPT processing of HEAs induces a transition from paramagnetic to ferromagnetic states at ambient conditions. This deformation-induced ferromagnetism can be explained by the cocktail effect in HEAs, where the formation of ferromagnetic particles is linked to deformation-induced element-selective atomic migration and local enrichment of ferromagnetic elements.

MM 37: Functional and Complex Materials

Time: Friday 12:00–12:45 Location: H22

MM 37.1 Fri 12:00 H22

Unveiling Material Dynamics with Machine-Learned Interatomic Potentials — •Ferenc Tasnadi, Bobur Mukhamedov, Amanda Ehn, Florian Trybel, and Igor A. Abrikosov — IFM Linköping University

Machine-learned interatomic potentials (MLIPs) have revolutionized our ability to understand the properties of materials with complex dynamical processes. In this work, we present an active learning MLIP strategy to: (i) investigate the elasticity of alloys near dynamical instability [1] and (ii) explore dynamical bond disorder in high-pressure synthesized PN2 [2]. bcc-Ti-based alloys have wide industrial applicability, ranging from low-modulus biomedical implants to high-strength GUM metals. The low-temperature dynamical instability of bcc-Ti can be tailored through the addition of bcc stabilizers (Nb, Ta, Zr, V), resulting in anomalous mechanical properties such as elinvar behavior or high anisotropy with low modulus in Ti-Nb-Zr and Ti-Zr-Sn alloys. Pnictogen compounds (Group 15 elements) exhibit fascinating chemistry due to the variety of bonding configurations, as demonstrated in the recently studied P-N system [2]. Long-timescale MLIP-driven simulations reveal that N-N distances connecting the P-N octahedra vary dynamically between single-bonded and non-bonding configurations. The results are compared with experimental observations. If time permits, we will demonstrate how MLIP-driven molecular dynamics simulations can offer deeper insights into materials exhibiting Peierls instability. [1] New J. Phys. 22 113005 (2020); J. Vac. Sci. Technol. A 42, 013412 (2024). [2] Chem. Eur. J. 2022, 28, e202201998.

MM 37.2 Fri 12:15 H22

Decoding Molecular Ion Dissociation Effects in Atom Probe Tomography of Iron Oxides — •Shyam Katnagallu[1], SeHo Kim[1], Shalini Bhatt[1], Daniel K Schreiber[2], Jörg Neugebauer[1], Baptiste Gault[1], and Christoph Freysoldt[1] — [1]Max Planck Institute for Sustainable Materials, Düsseldorf, Germany — [2]Energy and Environment Directorate, PNNL, Richland, USA.

To mitigate CO2 emissions, we require efficient carbon-free reduction processes for iron ores. Atom probe tomography (APT) can elucidate the gradual reduction of FexO at the nanometer length scale, but it is hindered by compositional bias. We investigated the changes in the measured composition of FeO, Fe2O3, and Fe3O4 across a range of analysis conditions. However, APT of ionic or covalently bonded materials often results in molecular ions. The metastability of these molecular ions, under an intense electrostatic field, makes them vulnerable to dissociation. These processes can significantly impact the analytical performance of APT. For instance, neutral molecules formed through dissociation may not be detected or may have a time-of-flight no longer associated with their actual mass, leading to their loss from the analysis. To predict possible dissociation reactions of molecular ions, we employed density-functional theory that considered the spin states of the molecules. The energetically favoured reactions were traced onto multi-hit correlation histograms to validate their existence within APT data. These detected reactions were carefully analysed to assess the impact of neutrals resulting from dissociation reactions on the performance of APT for analysing iron oxides.

MM 37.3 Fri 12:30 H22

Entropy Decoupling in Vacancy Formation of BCC High-Entropy Alloys — •Xiang Xu, Xi Zhang, and Blazej Grabowski — University of Stuttgart, Stuttgart, Germany

The temperature-dependent vacancy formation energies in MoTaNbW systems have been calculated using a machine-learning-based interatomic potential that accurately captures the simultaneous effects of configurational and vibrational entropies, along with their coupling. Our results indicate that at elevated temperatures, careful treatment of the chemical potential is essential. We computed the distributions of vacancy formation energies up to the melting point, explicitly accounting for anharmonic vibrational effects. The findings demonstrate that, in this system, the local atomic environment around a vacancy exerts minimal influence on the vibrational entropy contributions.